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Screening Level Ecological Risk Assessment Protocol for Hazardous Waste Combustion Facilities

Volume One

Peer Review Draft

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Volume One

U.S. EPA, OFFICE OF SOLID WASTE

U.S. ENVIRONMENTAL PROTECTION AGENCY

DISCLAIMER

This document provides guidance to U.S. EPA Regions and States on how best to implement RCRA and U.S. EPA's regulations to facilitate permitting decisions for hazardous waste combustion facilities. It also provides guidance to the public and to the regulated community on how U.S. EPA intends to exercise its discretion in implementing its regulations. The document does not substitute for U.S. EPA's regulations, nor is it a regulation itself. Thus, it cannot impose legally-binding requirements on U.S. EPA, States, or the regulated community. It may not apply to a particular situation based upon the circumstances. U.S. EPA may change this guidance in the future, as appropriate.

ACKNOWLEDGMENTS

Jeff Yurk (U.S. EPA Region 6), the primary author/editor of this document, would like to acknowledge that the development of this document could not have been accomplished without the support, input, and work of a multitude of U.S. EPA and support contractor personnel. The foundation for the combustion-related guidance and methodologies outlined in this document were first developed by the Office of Research and Development (ORD) and the Office of Solid Waste (OSW) in previous versions of combustion risk assessment guidance. The State of North Carolinas' combustion risk assessment methodology was also evaluated in preparation of this document. The foundation for the ecological risk-related procedures and methodologies outlined in this document were based on previous guidance developed by the Office of Research and Development (ORD) and EPA's Superfund program. This version of the protocol was originally initiated in response to the desire of the Region 6 Multimedia Planning and Permitting Division to implement an up-to-date and technically sound hazardous waste combustion permitting program. The decision to incorporate guidance on a full range of national combustion risk assessment issues into the document was encouraged and supported by the Director of the Office of Solid Waste.

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Contributions by Larry Johnson of the National Exposure Research Laboratory of ORD and Jeff Ryan and Paul Lemieux of the National Risk Management Research Laboratory of ORD were significant in providing methodologies for conducting TO analysis and defining appropriate detection limits to be used in the risk assessment. Donna Schwede of the National Exposure Research Laboratory of ORD and Jawad Touma of the Office of Air Quality Planning and Standards provided technical review comments to strengthen the air modeling section of the document. Review and comment on the soil and water fate and transport models was provided by Robert Ambrose of EPA's Environmental Research Laboratory in Athens, GA.

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Region 6 looks forward to the insight and input yet to be provided by the public and other interested parties during the full external peer review of the document.

REVIEWERS

Preliminary drafts of this ecological risk assessment document, as well as its companion human health risk assessment document, have received extensive internal Agency and State review. The following is a list of reviewers who have commented on these documents prior to their release as a peer review draft.

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TABLE OF CONTENTS

TABLE OF CONTENTS (Continued)

Chapter **Page**

TABLE OF CONTENTS (Continued)

TABLE OF CONTENTS (Continued)

TABLE OF CONTENTS (Continued)

TABLE OF CONTENTS (Continued)

TABLE OF CONTENTS (Continued)

APPENDICES

Appendix

FIGURES

TABLES

LIST OF ACRONYMS

µg	Microgram
µg/kg	Micrograms per kilogram
µg/L	Micrograms per liter
µg/s	Micrograms per second
µm	Micrometer
µm/s	Micrometers per second
μm^2	Square micrometers
^oC	Degrees Celsius
^oF	Degrees Fahrenheit
^oK	Degrees Kelvin
ADOM	Acid Deposition and Oxidant Model
AET	Apparent effects threshold
APCS	Air pollution control system
atm-m^3/mol-K	Atmosphere-cubic meters per mole-degrees Kelvin
ATSDR	Agency for Toxic Substances and Disease Registry
AWFCO	Automatic waste feed cutoff
AWQC	Ambient water quality criteria
BAF	Bioaccumulation factor
BaP	Benzo(a)pyrene
BCF	Bioconcentration factor
BD	Soil bulk density
BEF	Bioaccumulation equivalency factor
BEHP	Bis(2-ethylhexyl)phthalate
BIF	Boiler and industrial furnace
BPIP	Building profile input program
BS	Benthic solids
BSAF	Sediment bioaccumulation factor
BTAG	Biological Technical Assistance Group
BW	Body weight
CARB	California Air Resources Board
CAS	Chemical Abstracts Service
CERM	Conceptual ecological risk model
CKD	Cement kiln dust
COMPDEP	COMPLEX terrain model with DEPosition
COMPLEX I	COMPLEX terrain model, Version 1
COPC	Compound of potential concern
CPF	Cumulative probability density function
CRQL	Contract required quantitation limit
CWA	Clean Water Act

LIST OF ACRONYMS (Continued)

DEHP	Diethylhexylphthalate (same as Bis(2-ethylhexl)phthalate)
DEM	Digital Elevation Model
DNOP	Di(n)octylphthalate
DOE	U.S. Department of Energy
DQL	Data quality level
DRE	Destruction and removal efficiency
EDQL	Ecological data quality levels
EEL	Estimated exposure level
EPA	U.S. Environmental Protection Agency
EPC	Exposure point concentration
EQL	Estimated quantitation limit
EQP	Equilibrium partitioning
ERA	Ecological risk assessment
ERL	Effects range low
ERT	Environmental Research and Technology
ESP	Electrostatic precipitator
ESI	Ecological screening index
ESQ	Ecological screening quotient
FCM	Food chain multiplier
FWS	U.S. Fish and Wildlife Service
g/s	Grams per second
g/cm^3	Grams per cubic centimeter
g/m^3	Grams per cubic meter
GAQM	Guideline on Air Quality Models
GC	Gas chromatography
GEP	Good engineering practice
HBC	Hexachlorobenzene
$HgCl_2$	Mercuric chloride
HQ	Hazard quotient
HSDB	Hazardous substances data base
IDL	Instrument detection limit
IEM	Indirect exposure model
IRIS	Integrated risk information system
ISCST3	Industrial source complex short-term model
ISCSTDFT	Industrial Source Complex Short Term Draft
kg	Kilogram
kg/L	Kilograms per liter

LIST OF ACRONYMS (Continued)

L	Liter
LC_{50}	Lethal concentration to 50 percent of the test population
LCD	Local Climatological Data Annual Summary with Comparative Data
LD_{50}	Lethal dose to 50 percent of the test population
LEL	Lowest effect level
LFI	Log fill-in
LOAEL	Lowest observed adverse effect level
LOD	Level of detection
LOEL	Lowest observed effect level
m	Meter
m/s	Meters per second
mg	Milligram
mg/kg	Milligrams per kilogram
mg/kg/day	Milligrams per kilogram per day
mg/L	Milligrams per liter
mg/m^3	Milligrams per cubic meter
MACT	Maximum achievable control technology
MDL	Method detection limit
MLE	Maximum likelihood estimation
MPRM	Meterological Processor for Regulatory Models
MPTER	Air quality model for multiple point source gaussian dispersion algorithm with terrain adjustments
MPTER-DS	Air quality model for multiple point source gaussian dispersion algorithm with terrain adjustments including deposition and sedimentation
NC DEHNR	North Carolina Department of Environment, Health, and Natural Resources
NCDC	National Climatic Data Center
NCEA	National Center for Environmental Assessment
NEL	No effect level
NFI	Normal fill-in
NOAA	National Oceanic and Atmospheric Administration
NOAEL	No observed adverse effect level
NOEC	No observed effect concentration
NOEL	No observed effect level
NRC	U.S. Nuclear Regulatory Commission
NTIS	National technical information service
NWS	National weather service
OAQPS	Office of Air Quality Planning and Standards
OAQPS TTN	Office of Air Quality and Planning Standards and Technology Transfer Network
OC	Organic carbon
OCDD	Octachlorodibenzodioxin
ORD	Office of Research and Development
ORNL	Oak Ridge National Laboratory
OSW	Office of Solid Waste

LIST OF ACRONYMS (Continued)

OV	Deposition output values
PAH	Polycyclic aromatic hydrocarbon
PCB	Polychlorinated biphenyl
PCDD	Polychlorinated dibenzo(p)dioxin
PCDF	Polychlorinated dibenzofuran
PCRAMMET	Personal computer version of the meterological preprocessor for the old RAM program
PDF	Probability density function
PIC	Product of incomplete combustion
PM	Particulate matter
PM10	Particulate matter less than 10 micrometers in diameter
POHC	Principal organic hazardous constituent
PQL	Practical quantitation limit
PRC	PRC Environmental Management, Inc.
PU	Polyurethane
QA/QC	Quality assurance/Quality control
QAPjP	Quality assurance project plan
QSAR	Quantitative structure activity relationship
RCRA	Resource Conservation and Recovery Act
REACH	
RME	Reasonable maximum exposure
RTDM	Rough terrain diffusion model
RTDMDEP	Rough terrain diffusion model deposition
RTECS	Registry of Toxic Effects of Chemical Substances
SAMSON	Solar and Meterological Surface Observational Network
SCRAM BBS	Support Center for Regulatory Air Models Bulletin Board System
SFB	San Francisco Bay
SMDP	Scientific management decision point
SO	Source
SQL	Sample quantitation limit
SVOC	Semivolatile organic compound
TAL	Target analyte list
TCDD	Tetrachlorodibenzo(p)dioxin
TDA	Toluene diisocyanate
TEF	Toxicity equivalent factor
TG	Terrain grid
TIC	Tentatively identified compound
TL	Trophic level
TOC	Total organic carbon
TRV	Toxicity reference value
TSS	Total suspended solids

LIST OF ACRONYMS (Continued)

UF	Uncertainty factor
UFI	Uniform fill-in
USGS	U.S. Geological Survey
USLE	Universal soil loss equation
UTM	Universal transverse mercator
VOC	Volatile organic compound
watts/m^2	Watts per square meter
WRPLOT	Wind Rose PLOTing program

LIST OF VARIABLES

λ_z	=	Dimensionless viscous sublayer thickness (unitless)
μ_a	=	Viscosity of air (g/cm-s)
μ_w	=	Viscosity of water corresponding to water temperature (g/cm-s)
ρ_a	=	Air density (g/cm^3 or g/m^3)
ρ_s	=	Bed sediment density (kg/L)
ρ_w	=	Density of water corresponding to water temperature (g/cm^3)
θ	=	Temperature correction factor (unitless)
θ_{bs}	=	Bed sediment porosity (unitless)
θ_s	=	Soil volumetric water content (mL/cm^3 soil)
a	=	Empirical intercept coefficient (unitless)
A	=	Surface area of affected area (m^2)
b	=	Empirical slope coefficient (unitless)
BAF_l	=	Bioaccumulation factor reported on a lipid-normalized basis using the freely dissolved concentration of a chemical in the water (L/kg)
$BCF_{a/s}$	=	Aquatic-sediment bioconcentration factor (unitless)
BCF_l	=	Bioconcentration factor reported on a lipid-normalized basis using the freely dissolved concentration of a chemical in the water (L/kg)
$BCF_{Pi\text{-}H}$	=	Bioconcentration factor for plant-to-herbivore for *i*th plant food item (unitless)
BCF_i	=	Soil-to-soil invertebrate bioconcentration factor (unitless)
$BCF_{Pi\text{-}OM}$	=	Bioconcentration factor for plant-to-omnivore for *i*th plant food item (unitless)
$BCF_{S/BS\text{-}C}$	=	Bioconcentration factor for soil- or bed sediment-to-carnivore (unitless)
$BCF_{S/BS\text{-}H}$	=	Bioconcentration factor for soil-to-plant or bed sediment-to-plant (unitless)
$BCF_{W\text{-}C}$	=	Bioconcentration factor for water-to-carnivore (L/kg)
$BCF_{W\text{-}HM}$	=	Bioconcentration factor for water-to-herbivore (L/kg)
BCF_{WI}	=	Bioconcentration factor for water-to-invertebrate (L/kg)
BCF_r	=	Plant-soil biotransfer factor (unitless)
BD	=	Soil bulk density (g soil/cm^3 soil)
BMF_n	=	Biomagnification factor for *n*th trophic level
BS	=	Benthic solids concentration (kg/L or g/cm^3)
$BSAF$	=	Sediment bioaccumulation factor (unitless)
Bv	=	Air-to-plant biotransfer factor (µg COPC/g DW plant)/(µg COPC/g air)
BW	=	Body weight (kg)
C	=	USLE cover management factor (unitless)
C_{Ai}	=	COPC concentration in *i*th animal food item (mg/kg)
C_C	=	COPC concentration in carnivore (mg/kg)
C_d	=	Drag coefficient (unitless)
C_{dw}	=	Dissolved phase water concentration (mg/L)
C_F	=	COPC concentration in fish (mg/kg)
CFO_2	=	Correction factor for conversion to 4.5 percent O_2 (unitless)
C_{gen}	=	Generic chemical concentration (mg/kg or mg/L)
C_H	=	COPC concentration in herbivore (mg/kg)
C_i	=	Stack concentration of *i*th identified COPC (carbon basis) (mg/m^3)

LIST OF VARIABLES (Continued)

C_i	=	COPC concentration in *i*th plant or animal food item (mg COPC/kg)
C_I	=	COPC concentration in soil or benthic invertebrate (mg/kg)
C_{IW}	=	COPC concentration in soil or sediment interstitial water (mg/L)
C_M	=	COPC concentration in media (mg COPC/kg [soil, sediment] or mg COPC/L [water])
C_{OM}	=	COPC concentration in omnivore (mg/kg)
C_{Pi}	=	COPC concentration in *i*th plant food item (mg/kg)
C_{PREY}	=	Concentration in prey
C_{sed}	=	COPC concentration in bed sediment (g COPC/cm^3 sediment or mg COPC/kg sediment)
$C_{s/sed}$	=	COPC concentration in soil or bed sediment (mg/kg)
C_{TOC}	=	Stack concentration of TOC, including speciated and unspeciated compounds (mg/m^3)
C_{TP}	=	COPC concentration in terrestrial plants (mg COPC/kg WW)
C_{wctot}	=	Total COPC concentration in water column (mg/L)
C_{wtot}	=	Total water body COPC concentration (including water column and bed sediment) (g/m^3 or mg/L)
Cyp	=	Unitized yearly air concentration from particle phase (μg-s/g-m^3)
Cyv	=	Unitized yearly air concentration from vapor phase (μg s/g m^3)
Cywv	=	Unitized yearly watershed air concentration from vapor phase (µg-s/g-m^3)
D_1	=	Lower bound of a particle size density for a particular filter cut size
D_2	=	Upper bound of a particle size density for a particular filter cut size
D_a	=	Diffusivity of COPC in air (cm^2/s)
d_{bs}	=	Depth of upper benthic sediment layer (m)
DD_{TEQ}	=	Daily dose of 2,3,7,8-TCDD *TEQ* (μg/kg BW/d)
DD_i	=	Daily dose of *i*th congener (μg/kg BW/d)
D_{mean}	=	Mean particle size density for a particular filter cut size
Ds	=	Deposition term (mg/kg-yr)
D_w	=	Diffusivity of COPC in water (cm^2/s)
d_{wc}	=	Depth of water column (m)
Dyd	=	Unitzed yearly dry deposition rate of COPC (g/m^2-yr)
Dydp	=	Unitized yearly dry deposition from particle phase (s/m^2-yr)
Dytwp	=	Unitized yearly watershed total deposition (wet and dry) from particle phase (s/m^2-yr)
Dywp	=	Unitized yearly wet deposition from particle phase (s/m^2-yr)
Dywv	=	Unitized yearly wet deposition from vapor phase (s/m^2-yr)
Dywwv	=	Unitized yearly watershed wet deposition from vapor phase (s/m^2-yr)
d_z	=	Total water body depth (m)
E_v	=	Average annual evapotranspiration (cm/yr)
ER	=	Soil enrichment ratio (unitless)

LIST OF VARIABLES (Continued)

F_{Ai}	=	Fraction of diet consiting of *i*th animal food item (unitless)
f_{bs}	=	Fraction of total water body COPC concentration in benthic sediment (unitless)
FCM	=	Trophic level-specific food-chain multiplier (unitless)
FCM_{TLn}	=	Food chain multiplier for *n*th trophic level
$FCM_{TLn\text{-}Ai}$	=	Food chain multiplier for trophic level of *i*th animal food item (unitless)
FCM_{TL3}	=	Food chain multiplier for trophic level 3 (unitless)
f_{wc}	=	Fraction of total water body COPC concentration in the water column (unitless)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
F_{OC}	=	Fraction of organic carbon (unitless)
F_{Pi}	=	Fraction of diet consisting of *i*th plant food item (unitless)
Fw	=	Fraction of COPC wet deposition that adheres to plant surfaces (unitless)
H	=	Henry's law constant (atm-m^3/mol)
Ir_{MEDIUM}	=	Ingestion rate of soil, surface water, or sediment
I	=	Average annual irrigation (cm/yr)
IR	=	Ingestion rate (kg/day)
k	=	von Karman's constant (unitless)
K	=	USLE erodibility factor (ton/acre)
k_b	=	Benthic burial rate (yr^{-1})
K_G	=	Gas phase transfer coefficient (m/yr)
K_L	=	Liquid phase transfer coefficient (m/yr)
Kd_{bs}	=	Bed sediment/sediment pore water partition coefficient (L/kg or cm^3/g)
Kd_{ij}	=	Partition coefficient for COPC i associated with sorbing material j (unitless)
Kd_s	=	Soil-water partition coefficient (cm^3/g or mg/L)
Kd_{sw}	=	Suspended sediments/surface water partition coefficient (L/kg)
K_{oc}	=	Organic carbon partition coefficient (mg/L)
K_{ocj}	=	Sorbing material-independent organic carbon partition coefficient for COPC j
K_{ow}	=	Octanol-water partition coefficient (unitless)
kp	=	Plant surface loss coefficient (yr^{-1})
ks	=	COPC soil loss constant due to all processes (yr^{-1})
kse	=	COPC loss constant due to soil erosion (yr^{-1})
ksg	=	COPC loss constant due to biotic and abiotic degradation (yr^{-1})
ksl	=	COPC loss constant due to leaching (yr^{-1})
ksr	=	COPC loss constant due to runoff (yr^{-1})
ksv	=	COPC loss constant due to volatilization (yr^{-1})
kv	=	Water column volatilization rate constant (yr^{-1})
Kv	=	Overall transfer rate coefficient (m/yr)
k_{wt}	=	Overall total water body COPC dissipation rate constant (unitless)
L	=	Monin-Obukhov Length (m)

LIST OF VARIABLES (Continued)

L_{DEP}	=	Total (wet and dry) particle phase and wet vapor phase direct deposition load to water body (g/yr)
L_{dif}	=	Dry vapor phase diffusion load to water body (g/yr)
L_E	=	Soil erosion load (g/yr)
L_R	=	Runoff load from pervious surfaces (g/yr)
L_{RI}	=	Runoff load from impervious surfaces (g/yr)
L_T	=	Total COPC load to water body (g/yr)
LS	=	USLE length-slope factor (unitless)
MW	=	Molecular weight of COPC (g/mol)
OC_i	=	Organic carbon content of sorbing material *I* (unitless)
OV	=	Deposition output values
P	=	Average annual precipitation (cm/yr)
P_{Ai}	=	Proportion of *i*th animal food item in diet that is contaminated (unitless)
Pd	=	COPC concentration in plant due to to direct deposition (mg/kg WW)
PF	=	USLE supporting practice factor (unitless)
P_{Pi}	=	Proportion of *i*th plant food item in diet that is contaminated (unitless)
Pr	=	COPC concentration in plant due to root uptake (mg/kg WW)
$P_{S/BS}$	=	Proportion of soil or bed sediment in diet that is contaminated (unitless)
Pv	=	COPC concentration in plant due to air-to-plant transfer (mg/kg WW)
P_W	=	Proportion of water in diet that is contaminated (unitless)
Q	=	COPC emission rate (g/s)
Q_i	=	Emission rate of COPC *(i)* (g/s)
$Q_{i(adj)}$	=	Adjusted emission rate of COPC *(i)* (g/s)
Q_f	=	Anthropogenic heat flux (W/m^2)
Q_*	=	Net radiation absorbed (W/m^2)
r	=	Interception fraction-the fraction of material in rain intercepted by vegetation and initially retained (unitless)
R	=	Universal gas constant (atm-m^3/mol-K)
RO	=	Average annual runoff (cm/yr)
RF	=	USLE rainfall (or erosivity) factor (yr^{-1})
Sc	=	Average soil concentration over exposure duration (mg/kg)
Sc_{Tc}	=	Soil concentration at time *Tc* (mg/kg)
SD	=	Sediment delivery ratio (unitless)
SGC	=	COPC stack gas concentration as measured in the trial burn (µg/dscm)
SGF	=	Stack gas flow rate at 7 percent O_2 (dscm/s)
T_a	=	Ambient air temperature (K) = 298.1 K
Tp	=	Length of plant exposure to deposition per harvest of the edible portion of the *i*th plant group (yr)

LIST OF VARIABLES (Continued)

tD	=	Total time period over which deposition occurs (time period of combustion) (yr)
T_m	=	Melting point temperature (K)
TSS	=	Total suspended solids concentration (mg/L)
T_w	=	Water body temperature (K)
u	=	Current velocity (m/s)
V	=	Volume
Vdv	=	Dry deposition velocity (cm/s)
Vf_x	=	Average volumetric flow rate through water body (m^3/yr)
VG_{ag}	=	Empirical correction factor for aboveground produce (unitless)
VP	=	Vapor pressure (atm)
W	=	Average annual wind velocity (m/s)
WA_I	=	Area of impervious watershed receiving COPC deposition (m^2)
WA_L	=	Area of watershed receiving COPC deposition (m^2)
WA_w	=	Water body surface area (m^2)
X_e	=	Unit soil loss (kg/m^2-yr)
Yp	=	Standing crop biomass (productivity) (kg/m^2 DW)
Z_s	=	Soil mixing zone depth (cm)

CONVERSIONS

0.001	=	Units conversion factor (g/mg)
10^6	=	Units conversion factor (µg/g)
907.18	=	Units conversion factor (kg/ton)
3.1536×10^7	=	Conversion constant (s/year)
4,047	=	Units conversion factor (m^2/acre)
100	=	Units conversion factor (m^2-mg/cm^2-kg)
10^{-6}	=	Units conversion factor (g/µg)
0.12	=	Dry weight to wet weight (plants) conversion factor (unitless)

Chapter 1
Introduction

What's Covered in Chapter 1:

- Objective and Purpose
- Related Trial Burn Issues
- Reference Documents
- Overview of the Risk Assessment Process
- Relationship to U.S. EPA HHRAP
- Definitions

Risk assessment is a science used to evaluate the potential hazards to the environment that are attributable to emissions from hazardous waste combustion units. There is general guidance available regarding the general ecological risk assessment process including problem formulation, analysis, and risk characterization (U.S. EPA 1997c; 1998d). This document expands on that general guidance with respect to the ecological screening level procedures and provides a prescriptive tool to support permitting of hazardous waste burning combustion facilities under the Resource Conservation and Recovery Act (RCRA). It is not intended to be used to perform screening or baseline ecological risk assessments (ERA) in other areas of the RCRA program, such as corrective action.

The following definitions were adopted from *Superfund: Process for Designing and Conducting Ecological Risk Assessments. Interim Final* (U.S. EPA 1997c) and *Guidelines For Ecological Risk Assessment* (U.S. EPA 1998d), and identify key terms used throughout this guidance. Some of the terms are annotated with additional information to clarify the definition and explain its use in this protocol.

Area Use Factor: A ratio of an organism's home range, breeding range, or feeding and foraging range to the area of contamination of the assessment area.

Assessment Endpoint: An explicit expression of the environmental value that is to be protected; it includes both an ecological entity and specific attributes of that entity. The assessment endpoint in this protocol is used to link the risk assessment to management concerns and ultimately development of a protective RCRA operating permit. One or more assessment endpoints may be selected for performing a risk assessment.

Bioaccumulation: The net accumulation of a substance by an organism as a result of uptake directly from all environmental sources, including food. Bioaccumulation occurs through all exposure routes.

Bioaccumulation Factor (*BAF*): *BAF* represents the ratio of the concentration of a chemical to its concentration in a medium. The factor must be measured at steady-state when the rate of uptake is balanced by the rate of excretion. In this protocol a bioaccumulation factor (*BAF*) is estimated by multiplying a bioconcentration factor (*BCF*) by a food chain multiplier (FCM) derived based on the trophic level of the prey ingested by a measurement receptor.

Bioconcentration: A process by which there is a net accumulation of a chemical directly from an exposure medium into an organism.

Bioconcentration Factor (*BCF*): *BCF* represents the ratio of the concentration of a chemical in an aquatic organism to the concentration of the chemical in surface water, sediment, or soil. The factor must be measured at steady-state when the rate of uptake is balanced by the rate of excretion. BCFs are used in this protocol to estimate the body burden of a COPC in producers, primary consumers, and fish consumed by mid- or upper-trophic level measurement receptors.

Biomagnification: The process by which the concentration of some chemicals increase with increasing trophic level; that is, the concentration in a predator exceeds the concentration in its prey. In this protocol, a ratio of FCM's are used to account for biomagnification.

Biotransfer Factor: COPC accumulation factor between a food item and its consumer. In this protocol biotransfer factors are used to evaluate transport of contaminants in plants to mammals and birds.

Depuration: The loss of a compound from an ecological receptor as a result of any active or passive process.

Direct Uptake: Direct uptake is a term applied to producers, primary consumers, and detritivores. Direct uptake includes all exposure routes for aquatic receptors, benthic receptors, soil invertebrates, and terrestrial plants. Direct uptake is used in this manner because it is difficult, given feeding and habitat niches of these receptors and limited availability of empirical information, to discern the relative importance of exposure through ingestion, respiration, dermal uptake, or root uptake. In addition, toxicity tests (used as the basis of risk assessment toxicity reference values) on these receptors (except some aquatic fauna) usually do not make a distinction between exposure routes or tend to overemphasize or isolate a particular route.

Ecological Effects Assessment: A portion of the analysis phase of the risk assessment that evaluates the ability of a stressor to cause adverse effects under a particular set of circumstances. Toxicity reference values identified in ecological effects assessment are used in risk characterization.

Ecological Risk Assessment: The process that evaluates the likelihood that adverse ecological effects may occur or are occurring as a result of exposure to one or more stressors.

Ecological Screening Quotient (ESQ): A quotient used to assess risk during the risk assessment in which protective assumptions are used. Generally, the numerator is the reasonable worst-case COPC concentration at the point of exposure, and the denominator is the no-adverse-effects-based toxicity reference value.

Environmental Attribute: Characteristic of a food web functional group (e.g., herbivorous mammal) that is relevant to the ecosystem. Examples of environmental attributes include seed dispersal, decompositon, pollination, and food source.

Exposure Assessment: A portion of the analysis phase of ERA that evaluates the interaction of the stressor with one or more ecological components. Exposure can be expressed as co-occurrence or contact, depending on the stressor and ecological component involved. Information from the exposure assessment is used in risk characterization.

Exposure Pathway: A pathway by which a compound travels from a combustion facility to an ecological receptor. A complete exposure pathway occurs when a chemical enters or makes contact with an ecological receptor through one or more exposure routes.

Exposure Route: A point of contact or entry of a chemical from the environment into an organism. The exposure routes for terrestrial wildlife are ingestion, dermal absorption, and inhalation. The exposure routes for aquatic fauna are ingestion, dermal absorption, and respiration. The exposure routes for terrestrial plants are root absorption or foliar uptake. Exposure routes for aquatic plants are direct contact with water and sediments.

Food Chain: The transfer of food energy from the source in plants through a series of organisms with repeated eating and being eaten (Odum 1971).

Food Web: The interlocking patterns of food chains (Odum 1971).

Food-Chain Multiplier (FCM): The FCM is used to account for dietary uptake of a compound by an ecological receptor. It may be used to estimate a *BAF* from a *BCF* in the absence of reliable *BAF* data. The FCM values in Table 5-1 have been adopted from *Water Quality Guidance for the Great Lakes System* (U.S. EPA 1995j).

Guild: A group of species occupying a particular trophic level and exploiting a common resource base in a similar fashion (Root 1967).

Habitat: The physical environment in which a species is distributed. Habitat location depends on several factors, such as chemical conditions, physical conditions, vegetation, species eating strategy, and species nesting strategy. By analogy, the habitat is an organism's "address."

Measure of Effect: A measurable ecological characteristic that is related to the valued characteristic chosen as the assessment endpoint. It is the measure used to evaluate the response of the assessment endpoint when exposed to a chemical (U.S. EPA 1998d). This protocol proposes, for each class/guild, representative receptors (measurement receptors) for characterizing risk from exposure to compounds emitted from a combustion facility.

Measure of Effect: A measurable ecological characteristic that is related to the valued characteristic chosen as the assessment endpoint.

Measure of Exposure: A measurable stressor characteristic that is used to help quantify exposure.

Measurement Receptor: A species, population, community, or assemblage of communities (such as "aquatic life") used to characterize ecological risk to an assessment endpoint.

Problem Formulation: A systematic planning step that identifies the focus and scope of the risk assessment. Problem formulation includes ecosystem characterization, pathway analysis, assessment endpoint development, and measurement endpoint identification. Problem formulation results in the development of a problem statement that is addressed in the analysis step.

Scientific and Management Decision Point: A point during the risk assessment at which the risk assessor and risk manager discuss results. The risk manager determines whether the information is sufficient to arrive at a decision regarding the significance of the results and whether additional information is needed before proceeding forward in the risk assessment.

Special Ecological Area: Habitats and areas for which protection and special consideration has been conferred legislatively (federal or state), such as critical habitat for federally or state-designated endangered or threatened species. In characterizing media concentrations of COPCs, special emphasis is placed on estimating concentrations and, therefore, exposure potential, in sensitive areas.

Stressor: Any physical, chemical, or biological entity that can induce an adverse response.

Trophic Level: One of the successive levels of nourishment in a food web or food chain. Plant producers constitute the first (lowest) trophic level, and dominant carnivores constitute the last (highest) trophic level.

Uncertainty Factor: Quantitative values used to adjust toxicity values from laboratory toxicity tests to toxicity values representative of chronic no-observed-adverse-effect-levels (NOAELs). In this guidance, uncertainty factors (UF) are used to extrapolate from acute and subchronic test duration to chronic duration, and to extrapolate from point estimated (e.g., LD50) and lowest-observed-adverse-effect-level (LOAEL) endpoints to an NOAEL endpoint.

Uptake: Acquisition by an ecological receptor of a compound from the environment as a result of any active or passive process.

This Screening Level Ecological Risk Assessment Protocol (SLERAP) has been developed as national guidance to consolidate information presented in other risk assessment guidance and methodology documents previously prepared by U.S. EPA and state environmental agencies. In addition, this guidance also addresses issues that have been identified while conducting risk assessments for existing hazardous waste combustion units. The overall purpose of this document is to explain how ecological risk assessments should be performed at hazardous waste combustion facilities. This document is intended as

(1) guidance for personnel conducting risk assessments, and (2) an information resource for permit writers, risk managers, and community relations personnel.

The RCRA "omnibus" authority of §3005(c)(3) of RCRA, 42 U.S.C. §6925(c)(3) and 40 CFR §270.32(b)(2) gives the Agency both the authority and the responsibility to establish risk-based permit conditions on a case-by-case basis as necessary to protect human health and the environment. These risk-based site-specific permit conditions are in addition to the national technical standards required in the hazardous waste incinerator and boiler/industrial furnace regulations of 1981 and 1991, respectively. Often, the determination of whether or not a permit is sufficiently protective can be based on its conformance to the technical standards specified in the regulations. Since the time that the regulations for hazardous waste incinerators and boilers/industrial furnaces were issued, however, additional information became available which suggested that technical standards may not fully address potentially significant risks. For example, many studies (including the *Draft Health Reassessment of Dioxin-Like Compounds*, *Mercury Study Report to Congress*, *Risk Assessment Support to the Development of Technical Standards for Emissions from Combustion Units Burning Hazardous Wastes: Background Information Document*, and the *Waste Technologies Industries (WTI) Risk Assessment*) indicate that there can be significant risks from indirect exposure pathways (e.g., pathways other than direct inhalation). The food chain pathway appears to be particularly important for bioaccumulative pollutants which may be emitted from hazardous waste combustion units. In many cases, risks from indirect exposure may constitute the majority of the risk from a hazardous waste combustor. This key portion of the risk from hazardous waste combustor emissions was not directly taken into account when the hazardous waste combustion standards were developed. In addition, uncertainty remained regarding the types and quantities of non-dioxin products of incomplete combustion emitted from combustion units and the risks posed by these compounds.

As a result, until such time that the technical standards could be upgraded to more completely address potential risk from hazardous waste combustion, U.S. EPA recommended, pursuant to the "omnibus" authority, that site-specific risk assessments be performed for all combustion facilities as a part of the RCRA permitting process. Performance of a site-specific risk assessment can provide the information necessary to determine what, if any, additional permit conditions are necessary for each situation to ensure that operation of the combustion unit is protective of human health and the

environment. Under 40 C.F.R. §270.10(k), U.S. EPA may require a permit applicant to submit additional information (e.g., a site-specific risk assessment) that the Agency needs to establish permit conditions under the omnibus authority. In certain cases, the Agency may also seek additional testing or data under the authority of RCRA §3013 (where the presence or release of a hazardous waste "may present a substantial hazard to human health or the environment") and may issue an order requiring the facility to conduct monitoring, testing, analysis, and reporting. Any decision to add permit conditions based on a site-specific risk assessment under this authority must be justified in the administrative record for each facility, and the implementing agency should explain the basis for the conditions.

U.S. EPA promulgation of the Maximum Achievable Control Technology (MACT) standards for hazardous waste incinerators, cement kilns and light-weight aggregate kilns effectively upgraded the existing national technical standards for these combustion units. U.S. EPA intends to similarly upgrade the technical standards for other types of hazardous waste combustors in a later rulemaking. Since the MACT standards are more protective than the original standards for incinerators, cement kilns and light-weight aggregate kilns, U.S. EPA revised its earlier recommendation regarding site-specific risk assessments. As discussed in the preamble to the final MACT rule, U.S. EPA recommended that the permitting authority determine if a site-specific risk assessment is needed in addition to the MACT standards in order to meet the RCRA statutory obligation of protection of human health and the environment. For hazardous waste combustors not subject to the Phase I MACT standards, U.S. EPA continues to recommend that site-specific risk assessments be conducted as part of the RCRA permitting process. If the permitting authority determines a risk assessment is warranted, it should be conducted as part of the RCRA permitting process.

The permitting agency should consider several factors in its evaluation of the need to perform a risk assessment (human health and ecological). These factors include:

- whether any proposed or final regulatory standards exist that U.S. EPA has shown to be protective for site-specific receptors
- whether the facility is exceeding any final technical standards
- the current level of hazardous constituents being emitted by a facility, particularly in comparison to proposed or final technical standards, and to levels at other facilities where risks have been estimated
- the scope of waste minimization efforts and the status of implementation of a facility waste minimization plan

- particular site-specific considerations related to the exposure setting (such as physical, land use, presence of threatened or endangered species and special subpopulation characteristics) and the impact on potential risks
- the presence of significant ecological considerations (e.g., high background levels of a particular contaminant, proximity to a particular sensitive ecosystem)
- the presence of nearby off-site sources of pollutants
- the presence of other on-site sources of pollutants
- the hazardous constituents most likely to be found and those most likely to pose significant risk
- the identity, quantity, and toxicity of possible non-dioxin PICs
- the volume and types of wastes being burned
- the level of public interest and community involvement attributable to the facility

This list is by no means exhaustive, but is meant only to suggest significant factors that have thus far been identified. Others may be equally or more important.

The companion document of the SLERAP is the Human Health Risk Assessment Protocol (HHRAP) (U.S. EPA 1998c). U.S. EPA OSW has prepared these guidance documents as a resource to be used by authorized agencies developing risk assessment reports to support permitting decisions for facilities with hazardous waste combustion units.

1.1 OBJECTIVE AND PURPOSE

This protocol is a multipathway screening tool based on reasonable, protective assumptions about the potential for ecological receptors to be exposed to, and to be adversely affected by, compounds of potential concern (COPC) emitted from hazardous waste combustion facilities. The U.S. EPA OSW risk assessment process is a prescriptive analysis intended to be performed expeditiously using (1) measurement receptors representing food web-specific class/guilds and communities, and (2) readily available exposure and ecological effects information. To avoid the time-intensive and resource-consuming process of collecting site-specific information on numerous constituents, this guidance provides a process to obtain and evaluate various types of technical information that will enable a risk assessor to perform a risk assessment

relatively quickly. Additionally this guidance provides: (1) example food webs; (2) example measurement receptor natural history information; (3) fate and transport data, bioconcentration factors, and toxicity reference values for 38 COPCs. In lieu of this information, a facility may substitute site-specific information where appropriate and approved by the applicable permitting authority.

U.S. EPA OSW's objective is to present a user-friendly set of procedures for performing risk assessments, including (1) a complete explanation of the basis of those procedures, and (2) a comprehensive source of data needed to complete those procedures. The first volume of this document provides the explanation (Chapters 1 through 6); and the second and third volumes (Appendices A-H) provides the data sources. Appendix A presents compound-specific information necessary to complete the risk assessment. Appendix B presents equations for calculating media concentrations. Appendices C and D provide chemical and media-specific bioconcentration factors (BCFs). Appendix E provides toxicity reference values (TRVs) for 38 compounds of potential concern (COPCs) and several possible measurement receptors. Appendix F presents equations for calculating risk. Appendix G provides contact information for obtaining site-specific species information, and Appendix H provides toxicological profiles for 38 COPCs. Figure 1-1 summarizes the steps needed to complete a screening level ecological risk assessment.

Implementation of this guidance will demonstrate that developing defensible estimates of compound emission rates is one of the most important elements of the risk assessment. As described in Chapter 2, traditional trial burns conducted to measure destruction and removal efficiency (DRE) do not sufficiently characterize organic products of incomplete combustion (PIC) and metal emissions for use in performing risk assessments. In some instances, a facility or regulatory agency may want to perform a pretrial burn risk assessment, following the procedures outlined in this document, to ensure that sample collection times during the trial burn or risk burn are sufficient to collect the sample volumes needed to meet the detection limits required for the risk assessment. The decision to perform such an assessment should consider regulatory permitting schedules and other site-specific factors.

U.S. EPA OSW anticipates that ecological risk assessments will be completed for new and existing facilities as part of the permit application process. The SLERAP recommends a process for evaluating *reasonable*—not theoretical worst-case maximum—potential risks to receptors posed by emissions from RCRA regulated units. The use of existing and site-specific information early in, and throughout, the risk assessment process is encouraged; protective assumptions should be made only when needed to ensure that

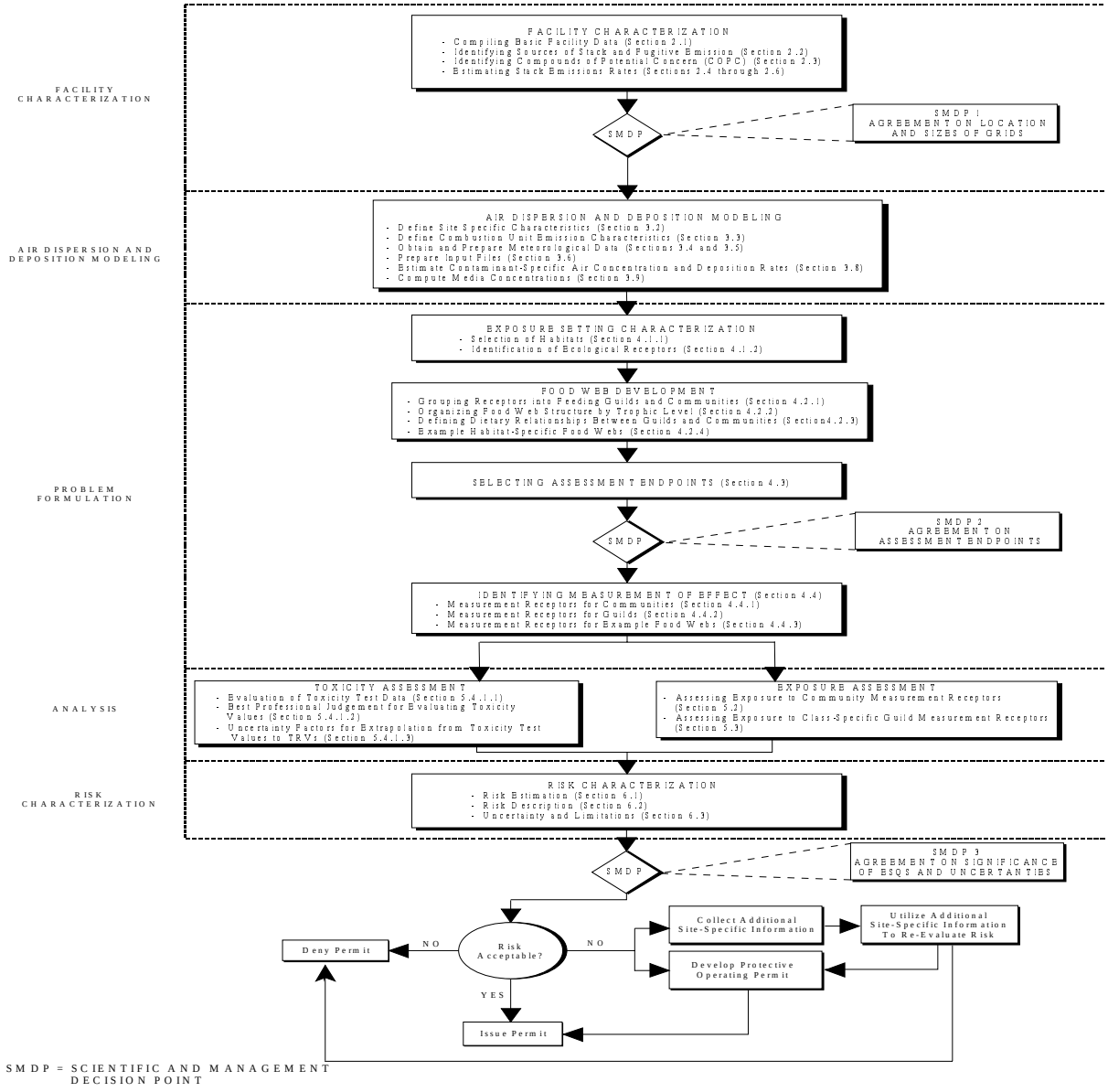
emissions from combustion units do not pose unacceptable risks. More protective assumptions may be incorporated to make the process fit a classical "screening level" approach that is more protective and may be easier to complete.

Regardless of whether theoretical worst case or more reasonable protective assumptions are used in completing the risk assessment process, every risk assessment is limited by the quantity and quality of:

- site-specific environmental data
- emission rate information
- other assumptions made during the risk estimation process (for example, fate and transport variables, exposure assumptions, and receptor characteristics)

These limitations and uncertainties are described throughout this document and the appendixes, and are summarized in Chapter 6.

FIGURE 1-1
SCREENING-LEVEL ECOLOGICAL RISK ASSESSMENT PROCESS



Potentially, unacceptable risks or other significant issues identified by collecting preliminary site information and completing risk assessment calculations can be addressed by the permitting process or during an iteration of the risk assessment. After the initial ecological risk assessment has been completed, it may be used by risk managers and permit writers in several ways:

- If the initial risk assessment indicates that estimated ecological risks are below regulatory levels of concern, risk managers and permit writers will likely proceed through the permitting process without adding any risk-based unit operating conditions to the permit.

- If the initial ecological risk assessment indicates potentially unacceptable risks, additional site-specific information demonstrated to be more representative of the exposure setting may be collected and additional iterations of risk assessment calculations can then be performed.

- If the initial risk assessment or subsequent iterations indicate potentially unacceptable risks, risk managers and permit writers may use the results of the risk assessment to revise tentative permit conditions (for example, waste feed limitations, process operating conditions, and expanded environmental monitoring). To determine if the subject hazardous waste combustion unit can be operated in a manner that is protective of the environment, an additional iteration of the risk assessment should be completed using the revised tentative operating conditions. If the revised conditions still indicate unacceptable risks, this process can be continued in an iterative fashion until acceptable levels are reached. In some situations, it may be possible to select target risk levels and back-calculate the risk assessment to determine the appropriate emission and waste feed rate levels. In any case, the acceptable waste feed rate and other appropriate conditions can then be incorporated as additional permit conditions.

- If the initial ecological risk assessment, or subsequent iterations, indicate potentially unacceptable risks, risk managers and permit writers may also choose to deny the permit.

This process is also outlined in Figure 1-1. As stated earlier, in some instances, a facility or regulatory agency may want to perform a pretrial burn risk assessment—following the procedures outlined in this document—to ensure that sample collection times during the trial burn or risk burn are sufficient to collect the sample volumes necessary to meet the appropriate detection limits for the risk assessment. This is expected to reduce the need for additional trial burn tests or iterations of the risk assessment due to problems caused when detection limits are not low enough to estimate risk with certainty sufficient for regulatory decision making.

1.2 RELATED TRIAL BURN ISSUES

In the course of developing this guidance and completing risk assessments across the country, U.S. EPA OSW has learned that developing defensible estimates of compound of potential concern (COPC) emission rates is one of the most important parts of the risk assessment process. As described in Chapter 2, traditional trial burns conducted to measure destruction and removal efficiency (DRE) *do not* sufficiently characterize organic products of incomplete combustion (PIC) and metal emissions for use in performing risk assessments.

U.S. EPA OSW considers the trial burn and risk assessment planning and implementation processes as interdependent aspects of the hazardous waste combustion unit permitting process. In addition, U.S. EPA OSW advocates that facility planning, regulatory agency review, and completion of tasks needed for both processes be conducted simultaneously to eliminate redundancy or the need to repeat activities. U.S. EPA OSW expects that the following guidance documents will typically be used as the main sources of information for developing and conducting appropriate trial burns:

- U.S. EPA. 1989f. *Handbook: Guidance on Setting Permit Conditions and Reporting Trial Burn Results. Volume II of the Hazardous Waste Incineration Guidance Series.* Office of Research and Development (ORD). EPA/625/6-89/019. January.
- U.S. EPA. 1989g. *Handbook: Hazardous Waste Incineration Measurement Guidance Manual. Volume III of the Hazardous Waste Incineration Guidance Series.* Office of Solid Waste and Emergency Response (OSWER). EPA/625/6-89/021. June.
- U.S. EPA. 1992e. *Technical Implementation Document for EPA's Boiler and Industrial Furnace Regulations.* OSWER. EPA-530-R-92-011. March.
- U.S. EPA. 1994n. *Draft Revision of Guidance on Trial Burns. Attachment B, Draft Exposure Assessment Guidance for Resource Conservation and Recovery Act (RCRA) Hazardous Waste Combustion Facilities*. OSWER. April 15.
- U.S. EPA. 1998b. *Guidance on Collection of Emissions Data to Support Site-Specific Risk Assessments at Hazardous Waste Combustion Facilities*. Prepared by EPA Region 4 and the Office of Solid Waste.
- Generic Trial Burn Plan and QAPPs developed by EPA regional offices or states.

1.3 REFERENCE DOCUMENTS

This section describes, in chronological order, the primary guidance documents used to prepare this guidance. Some of the guidance documents received a thorough review from EPA's Science Advisory Board, which mostly supported the work. Additional references used to prepare this guidance are listed in the References chapter of this document. These documents have been developed over a period of several years; in most cases, revisions to the original guidance documents address only the specific issues being revised rather than representing a complete revision of the original document. The following discussion lists and briefly describes each document. Overall, each of the guidance documents reflects a continual enhancing of the methodology.

This ecological assessment portion of this protocol is based on protecting the functions of ecological receptors in ecosystems and protecting special ecological areas around a hazardous waste combustion facility. It is generally consistent with current U.S. EPA guidance, including the Risk Assessment Forum's *Guidelines for Ecological Risk Assessment* (U.S. EPA 1998d), as well as the interim final *Ecological Risk Assessment Guidance for Superfund* (U.S. EPA 1997c) The most current methodology for assessing fate and transport of COPC's frequently referenced in this guidance is the U.S. EPA document, *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (In Press).

The following document was the first U.S. EPA NCEA guidance document for conducting risk assessments at combustion units:

- U.S. EPA. 1990a. *Interim Final Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. Environmental Criteria and Assessment Office. ORD. EPA-600-90-003. January.

This document outlined and explained a set of general procedures recommended in this guidance for determining media concentrations utilized in ecological risk assessments. This document was subsequently revised by the following:

- U.S. EPA. 1993h. *Review Draft Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. Office of Health and Environmental Assessment. ORD. EPA-600-AP-93-003. November 10.

U.S. EPA (1993h) outlined recommended revisions to previous U.S. EPA guidance (1990a), which have been used by the risk assessment community since the release of the document; however, these recommended revisions were never formally incorporated into the original document.

Finally, U.S. EPA Region 5 contracted for development of a *Screening Ecological Risk Assessment of Waste Technologies Industries (WTI) Hazardous Waste Incinerator*, in Liverpool, Ohio (U.S. EPA 1995l). This document was extensively peer reviewed and represents the most current application of ecological risk assessment guidance at a combustion facility. The WTI screening ecological risk assessment was reviewed and considered throughout the development of the approach presented in this guidance document.

U.S. EPA. 1998d. *Proposed Guidance for Ecological Risk Assessment*. Risk Assessment Forum, Washington, D.C. EPA/630/R-95/002B. August.

U.S. EPA. 1997c. *Ecological Risk Assessment Guidance for Superfund: Process for Designing and Conducting Ecological Risk Assessments*. Interim Final. Environmental Response Team, Office of Emergency and Remedial Response, Edison, New Jersey. June 5.

Root, R.B. 1967. "The Niche Exploitation Pattern of the Blue-Gray Gnatcatcher." *Ecological Monographs*. Volume 37, Pages 317-350.

Odum, E.P. 1971. *Fundamentals of Ecology*. Third Edition. W.B. Saunders Company, Philadelphia. 574 pp.

Chapter 2
Facility Characterization

What's Covered in Chapter 2:

- Compiling Basic Facility Information
- Identifying Emission Sources
- Estimating Emission Rates
- Identifying Compounds of Potential Concern (COPCs)
- Estimating COPC Concentrations for Non-Detects
- Evaluating Contamination In Blanks

This chapter provides guidance on characterizing the nature and magnitude of emissions released from facility sources. The characterization includes (1) compiling basic facility information, (2) identifying emission sources, (3) estimating emission rates, (4) identifying COPCs, (5) estimating COPC concentrations for non-detects, and (6) evaluating contamination in blanks.

2.1 COMPILING BASIC FACILITY INFORMATION

Basic facility information should be considered in conducting the risk evaluation, and provided to enable reviewers to establish a contextual sense of the facility regarding how it relates to other facilities and other hazardous waste combustion units. At a minimum, the basic facility information listed in the highlighted box at the end of this and other sections should be considered in the risk evaluation. The following sections and chapters describe the collection of this information in more detail; however, users may want to consult these discussions so that all site-specific information needed to complete the risk assessment can be collected simultaneously, when appropriate, for up front consideration. The risk assessor is also referred to *Briefing the BTAG: Initial Description of Setting, History, and Ecology of a Site* (U.S. EPA 1992a) (see web site www.epa.gov/superfund/program/risk/tooleco.htm) for more guidance on compiling basic facility information.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Principal business and primary production processes
- Normal and maximum production rates
- Types of waste storage and treatment facilities
- Type and quantity of wastes stored and treated
- Process flow diagrams showing both mass and energy inputs and outputs
- Type of air pollution control system (APCS) associated with each unit

2.2 IDENTIFYING EMISSION SOURCES

Combustion of a hazardous waste generally results in combustion by-products being emitted from a stack. In addition to emissions from the combustion stack, additional types of emissions of concern that may be associated with the combustion of hazardous waste include (1) process upsets, (2) general RCRA fugitive emissions, (3) cement kiln dust (CKD) fugitive emissions, and (4) accidental releases. Each of these emission source types are defined below with regards to the context and scope of this guidance.

Stack Emissions - Release of compounds or pollutants from a hazardous waste combustion unit into the ambient air while the unit is operated as intended by the facility and in compliance with a permit and/or regulation (for interim status).

Process Upset Emissions - Release of compounds or pollutants from a hazardous waste combustion unit into the ambient air while the unit is not being operated as intended, or during periods of startup or shutdown. Upset emissions usually result from an upset in the hazardous waste combustion process and are often known as process upset emissions. Upset emissions are generally expected to be greater than stack emissions because the process upset results in incomplete destruction of the wastes or other physical or chemical conditions within the combustion system that promote the formation and/or release of hazardous compounds from combustion stacks. Upset emissions usually occur during events and times when the hazardous waste combustion unit is not operating within the limits specified in a permit or regulation.

RCRA Fugitive Emissions - Release of compounds or pollutants into the ambient air from RCRA regulated sources other than hazardous waste combustion stacks. RCRA fugitive emissions are typically associated with the release of compounds or pollutants from leaks in the combustion

chamber (e.g., "puffs"); tanks, valves, flanges, and other material handling equipment used in the storage and handling of RCRA hazardous wastes; residues from the combustion process such as ash or quench water; and other RCRA treatment, storage, or disposal units (e.g., landfills).

CKD Fugitive Emissions - Release of compounds or pollutants into the ambient air caused by the handling, storage, and disposal of cement kiln dust.

Accidental Release - Accidental release is defined in Section 112(r) of the Clean Air Act as an unanticipated emission of a regulated substance or other extremely hazardous substance into the ambient air from a stationary source. Accidental releases are typically associated with non-routine emissions from RCRA facilities; such as the failure of tanks or other material storage and handling equipment, or transportation accidents.

Consistent with previous U.S. EPA guidance (U.S. EPA 1994d), U.S. EPA OSW recommends that, with the exception of accidental releases, all of these emission source types be addressed in the risk assessment, as applicable. Accidental releases are not considered within the scope of this guidance, and should be evaluated as recommended in Section 112(r) of the CAA and current U.S. EPA guidance (U.S. EPA 1996k) or the *RMP Offsite Consequence Analysis Guidance*, dated May 24, 1996. A decision to consider accidental releases in risk assessments for hazardous waste combustion facilities should be made on a site specific basis by the relevant permitting authority.

The following subsections contain guidance for estimating emissions for the source types specified for inclusion in the risk assessment. Guidance on air dispersion modeling of stack and fugitive emissions is presented in Chapter 3.

2.2.1 Estimating Stack Emission Rates for Existing Facilities

Stack emission rates (in grams per second) need to be determined for every compound of potential concern (COPC) identified using the procedures outlined in Section 2.3. U.S. EPA OSW expects that emission rates used to complete the risk assessment will be (1) long-term average emission rates adjusted for upsets, or (2) reasonable maximum emission rates measured during trial burn conditions in order to assure that risk assessments are conservative. Maximum emission rates measured during trial burn conditions (see Section 2.2.1.1) represent reasonable maximum emission rates. These emission rates can be controlled by hourly rolling average permit limits traditionally found in combustion unit operating permits, and are more conservative than emission estimates that are based on long-term average emission rates. Long-term

average emission rates (see Section 2.2.1.2) are based on tests of the combustion unit burning worst-case wastes at operating conditions that are representative of normal operating conditions over a long-term period. If long-term average emission rate estimates are used in the risk assessment, the final permit will likely specify limitations in addition to any hourly rolling average limit typically used to regulate hazardous waste combustion facilities.

A permitting agency's decision to allow a facility to use emission rate data developed from either normal or maximum operating conditions will be made on a case-by-case basis. Some facilities may be required to use emission rate data developed from maximum operating conditions because the variability in waste feed and operating conditions is too great to make permit decisions based on emission data collected during normal operating conditions, or because the emissions from combustion of the waste feed material are anticipated to be highly toxic and only a conservative risk assessment can adequately ensure protection.

2.2.1.1 Estimates from Trial Burns

For existing facilities (such as those built and operational), emission rate information will generally be determined by direct stack measurements during pretrial burn or trial burn tests, because trial burn tests are generally part of the permitting process to burn hazardous wastes. This policy is consistent with U.S. EPA 1998 *Guidance on Collection of Emissions Data to Support Site-Specific Risk Assessments at Hazardous Waste Combustion Facilities*, prepared by U.S. EPA Region 4 and OSW (U.S. EPA 1998b). For new facilities (see Section 2.2.3), estimated emission rates used to complete pretrial burn risk assessments should be compared to the emission rates estimated from actual trial burns completed after the new facility receives a permit and is constructed. Trial burn tests are designed to produce emission rates higher than those anticipated under normal operating conditions. U.S. EPA OSW recommends that sampling be conducted, in accordance with U.S. EPA guidance on conducting trial burns, by using compound-specific stack sampling, analytical, and quality assurance/quality control (QA/QC) protocols and procedures approved by the permitting authority. An alternative to a trial burn test is the submittal of data "in lieu of" a trial burn. U.S. EPA OSW will consider this type of data for on-site units on a case-by-case basis. U.S. EPA OSW expects that this data to be based on recent stack test measurements from a similar type of combustion unit with similar waste feed, capacity, operating conditions, and air pollution control systems (APCSs) to ensure comparable emission rates and destruction and removal efficiencies (DREs).

U.S. EPA OSW expects that using data from a trial burn as a basis for estimating COPC emission rates will tend to overestimate risk. COPC emission rates measured during trial burns are expected to be greater than emission rates during normal unit operations, because a facility "challenges" its combustion unit during a trial burn to develop a wide range of conditions for automatic waste feed cutoff (AWFCO) systems. Trial burn tests are usually conducted under two conditions: (1) a high-temperature test, in which the emission rate of metals is maximized, and (2) a low-temperature test, in which the ability of the combustion unit to destroy principal organic hazardous constituents (POHCs) in the waste feed is challenged. The lessor of the 95th percentile of the mean or maximum stack gas concentration from the three trial burn runs should be used to develop the emission rate estimate used in the risk assessment.

High POHC feed rates and extreme operating conditions tested during the low-temperature trial burn test are usually expected to result in greater product of incomplete combustion (PIC) emission rates. However, this is not true in all cases. For example, the formation of PCDDs and PCDFs does not necessarily depend on "POHC incinerability" low temperature conditions. Polychlorinated dibenzo(p)dioxins (PCDDs) and polychlorinated dibenzofurans (PCDFs) can be formed as a result of (1) catalytic formation in the low-temperature regions of the combustion unit or APCS during the low temperature test, or (2) catalytic formation that is dependent on high APCS temperatures typically experienced during the high temperature test.

Because the amount of testing required to develop estimates of COPC emission rates is so extensive and time consuming, U.S. EPA OSW places the responsibility for selecting the test conditions first on the facility and then on the permit writer. If a facility desires to receive a permit with no limits other than those traditionally based on hourly rolling average data gathered during a trial burn, then risk testing should be conducted during trial burn or "worst case" conditions. Whether the permit writer requires testing to be conducted at low, high, or both temperature conditions is a decision that must be made by the permit writer based on the characteristics of the facility and policy set forth by the senior management of the appropriate regulatory agency.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- All (current and historical) stack sampling information regarding rates of emissions from the combustion unit during normal or trial burn conditions
- Description of the waste feed streams burned during the stack sampling, including chemical composition and physical properties, which demonstrate that the waste feeds are representative of worst case site-specific "real" wastes

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Although U.S. EPA OSW will not require a risk assessment for every possible metal or PIC from a combustion unit, this does not imply that U.S. EPA OSW will allow only targeted sampling for COPCs during trial burn tests. Based on regional permitting experience and discussions with regional analytical laboratories, U.S. EPA OSW maintains that complete target analyte list analyses conducted when using U.S. EPA standard sampling methods (e.g., 0010 or 0030), do not subject facilities to significant additional costs or burdens during the trial burn process. Facilities conducting stack emission sampling should strive to collect as much information as possible which characterizes the stack gases generated from the combustion of hazardous waste. Therefore, every trial burn or "risk burn" should include, at a minimum, the following tests: Method 0010, Method 0030 or 0031 (as appropriate), total organic compounds (using the Guidance for Total Organics, including Method 0040), Method 23A, and the multiple metals train. Other test methods may be approved by the permitting authority for use in the trial burn to address detection limit or other site-specific issues.

2.2.1.2 Normal Operation Emission Rate Data

Facilities with limited waste feed characteristics and operational variability may be allowed to conduct risk testing at normal operational conditions (U.S. EPA 1994c). The collection of COPC data during normal operating conditions is referred to as a “risk burn” throughout the remainder of this guidance. It is important to note, however, that a risk burn does not replace a traditional trial burn conducted to measure DRE. Instead, U.S. EPA OSW considers a risk burn as an additional operating condition of the trial burn during which data is collected for the purpose of completing a risk assessment.

Because operational data collected during the risk burn would not normally be extrapolated to hourly rolling average AWFCO limits specified in an operating permit; the regulatory agency permit writer should

craft the permit with conditions designed to ensure that the facility does not operate at conditions in "excess" of the normal conditions over the long-term operation of the facility (for example, waste feed rate or stack gas flowrate). These additional permit limits are anticipated to take the form of quarterly or annual mass feed limitations on the waste feed, quarterly or annual average temperatures or stack gas flow rates, and other appropriate limitations.

It may also be necessary for the permit to contain appropriate reporting requirements to ensure that the regulatory agency can verify that the facility does not normally operate at conditions in excess of those tested during the risk burn. Monthly, quarterly, or annual reports which document long-term operations will likely be required of the facility. If a facility violates a long-term permit condition, the permit writer may also include language that requires the facility to cease waste burning immediately until a new test, risk assessment, and/or revised permit are completed. More detailed guidance on the development of permit limits can be found in U.S. EPA Region 6's *Hazardous Waste Combustion Permitting Manual*; which can be obtained from the U.S. EPA Region 6 web page (www.epa.gov/region06/).

One of the most important criteria which should be evaluated when considering the collection of data during a risk burn rather than a trial burn is the ability of the facility to document that the test is conducted with "worst case" waste. Worst case waste should be the waste feed material or combination of materials that are most likely to result in significant emissions of COPCs. The potential for both PIC and metal emissions should be considered in the selection of the worst case waste. For example, if a facility burns two types of waste—one waste with a high chlorine content and a significant concentration of aromatic organic compounds and a second with a low chlorine content and a significant concentration of alkanes—the former waste should be considered to be the "worst case" for PIC formation and should be used during the risk burn. A similar evaluation should be considered when selecting the worst case waste for metal emissions.

If a facility chooses to develop—and the appropriate regulatory agency allows the use of—emission rate estimates from a risk burn rather than a trial burn, the data set for each COPC should be the 95th percentile of the mean COPC emission rate over all the acceptable test runs *or* the maximum COPC emission rate value from all acceptable test runs, whichever value is lower. U.S. EPA OSW does not believe that it is reasonable to perform a risk assessment with the 95th percentile of the mean emission rate

if the maximum rate is less than this value. U.S. EPA OSW also recommends that, where possible, the COPC emission rate value from the trial burn test and the risk burn test be compared in the risk assessment report along with a comparison of the operational conditions at these two test conditions. For example, if the POHC used for the DRE test in the trial burn is a semivolatile organic compound (SVOC), the facility should analyze for all SVOCs (Method 0010) during the trial burn, and compare these values to those reported for the risk burn. The difference between the emission rates from the trial burn and risk burn should be evaluated in the uncertainty section of the risk assessment.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Sampling and analytical data for trial burn and risk burn (if the risk assessment is completed by using risk burn data) operating conditions
- Description of the operating conditions, under which each set of emission rate data being used was developed
- Complete evaluation of the differences between trial burn and risk burn operating conditions, with an explanation of the expected resultant risk differences

2.2.1.3 Estimates of the Total Organic Emission (TOE) Rate

Organic compounds that cannot be identified by laboratory analysis will not be treated as COPC's in the risk calculations. However, these compounds still may contribute significantly to the overall risk, and therefore, should be considered in the risk assessment (DeCicco 1995; U.S. EPA 1994d). U.S. EPA developed the total organic emissions (TOE) test to account for unidentified organic compounds because existing methods, such as total hydrocarbon analyzers, do not fully determine the total mass of organics present in stack gas emissions (Johnson 1996). U.S. EPA OSW anticipates that trial and risk burns will include sampling for TOE in order to provide permitting authorities with the information needed to address concerns about the unknown fraction organic emissions. The TOE can be used in conjunction with the identified organic compounds to calculate a TOE factor which can then be used to facilitate a evaluation of potential risks from the unidentified fraction of organic compounds in the stack gas.

The TOE test is the subject of other guidance; see the *Guidance for Total Organics* (U.S. EPA 1996b).

Use of the TOE data is dependent on a good understanding of the test method and how the data is reported.

The TOE method defines total organics as the sum of three fractions:

Fraction 1: **Total Volatile Organic Compounds (TO_{VOC}) (referred to as Field GC Component in the TO Guidance)** - TO_{VOC} is defined as the fraction of organic compounds having a boiling point less than 100°C. This VOC fraction is collected using U.S. EPA Method 0040. U.S. EPA Method 0040 allows for quantification of the total mass of organic compounds with boiling points less than 100°C, determined by summing the gas chromatograph/flame ionization detector results as described in the TO Guidance.

Fraction 2: **Total Chromatographical Semivolatiles (TO_{SVOC}) (referred to as Total Chromatographical Organics Component in the TO Guidance)** - TO_{SVOC} is defined as the fraction of organic compounds having boiling points between 100°C and 300°C. This VOC fraction is collected using modified U.S. EPA Method 0010 procedures as defined by U.S. EPA (1996b). The total mass of organic compounds with boiling points 100°C to 300°C is determined by summing the total gas chromatorgraph/flame ionization detector results as described in the TO Guidance.

Fraction 3: **Total Gravimetric Compounds (TO_{GRAV}) (referred to as Gravametric component in the TO Guidance)** - TO_{GRAV} is defined as the fraction of organic compounds having boiling points greater than 300°C. This fraction includes two types of compounds: (1) Identified SVOCs collected using U.S. EPA Method 0010 having boiling points greater than 300°C and (2) unidentified nonvolatile organics having boiling points greater than 300°C. This fraction is determined by using modified U.S. EPA Method 0010 procedures defined by U.S. EPA (1996b), which quantifies the mass, above this fractions boiling point, by measuring the total mass by evaporation and gravimetry (weighing) for nonvolatile total organics.

It should be noted that the TO total (TO_{TOTAL}) is the sum of the sums of each fraction. The sum of the TO fractions are described as follows:

$$TO_{TOTAL} = TO_{VOC} + TO_{SVOC} + TO_{GRAV} \qquad \text{Equation 2-1}$$

where

TO_{TOTAL}	=	stack concentration of TO, including identified and unidentified compounds (mg/m^3)
TO_{VOC}	=	stack concentration of volatile TO, including identified and unidentified compounds (mg/m^3)

TO_{SVOC}	=	stack concentration of SVOC TO, including identified and unidentified compounds (mg/m^3)
TO_{GRAV}	=	stack concentration of GRAV TO, including identified and unidentified compounds (mg/m^3)

The TOE data is used in conjunction with the identified data to compute a TOE factor. TOE factors have been computed which range from 2 to 40. The TOE factor is defined by this guidance as the ratio of the TO_{TOTAL} mass to the mass of identified organic compounds and calculated by the following equation:

$$F_{TOE} = \frac{TO_{TOTAL}}{\sum_i C_i} \qquad \text{Equation 2-2}$$

where

F_{TOE}	=	TOE factor (unitless)
TO_{TOTAL}	=	total organic emission (mg/m^3)
C_i	=	stack concentration of the *i*th identified COPC (mg/m^3)

One of the most critical components of the TOE factor is the identification of the organic compounds in the denominator of Equation 2-2. Although the permitting authority may not require a facility to analyze the organic compounds with all possible analytical methods, facilities should consider the effects that gaps in compound specific identification may have on the computation of the TOE factor. For example, hazardous waste burning cement kilns have expressed concern about the amount of light hydrocarbons that may be evolved from the raw materials processed in the cement kilns because these light hydrocarbons have not typically been identified in trial burns. If such concerns are significant, permitting authorities and facilities may choose to use additional test methods in the trial burn in order to speciate the maximum number of organic compounds.

U.S. EPA OSW also recommends that permitting authorities include tentatively identified compounds (TICs) in the denominator when computing the TOE factor to ensure that appropriate credit is given to defensible efforts at identifying the maximum number of organic compounds. Finally, U.S. EPA OSW recommends that non-detect compounds of potential concern be treated consistently between the risk assessment and TOE evaluation. That is, if a non-detected constituent is deleted as a compound of

potential concern (See Section 2.3), then it would not be included in the identified fraction of the TOE equation. Compounds of potential concern identified as per Section 2.3, but not detected, should be included in the TOE factor equation at the reliable detection limit (non-isotope dilution methods) or the estimated detection limit (isotope dilution methods).

The results of the gravimetric fraction should also be carefully evaluated when using the TOE factor. Both regulated industry and U.S. EPA scientists have expressed some concern that the gravimetric fraction of TOE test may contain materials that are not organic. U.S. EPA Office of Research and Development National Risk Management Research Laboratory (NRMRL) recently completed a study conducted to identify products of incomplete combustion (U.S. EPA 1997a). U.S. EPA NRMRL suggested in the study report that the gravimetric fraction of the TOE test may consist of organic and/or inorganic mass not directly attributable to organic incinerator emissions. U.S. EPA NRMRL theorized that these artifacts could consist of inorganic salts, super-fine particulate, or fractured XAD-2 resin. U.S. EPA NRMRL also concluded in this study report that the vast majority of the non-target semivolatile organic compounds detected, but not fully identified, were alkanes with more than 10 carbon atoms, esters of high molecular weight carboxylic acids, and phthlates. Most problems associated with accurately determining the gravimetric fraction attributable to incinerator emissions can be minimized; see the U.S. EPA 1998 *Guidance on Collection of Emissions Data to Support Site-Specific Risk Assessments at Hazardous Waste Combustion Facilities* (U.S. EPA 1998b) for minimizing sample errors.

The TOE factor is used in the uncertainty section of the risk assessment report to evaluate the risks from the unknown fraction of organics. Permitting authorities can evaluate the TOE factor and assess to what extent actual risks may be greater than estimated risks. For example, if the risk from the known portion of the emissions show that risks may be borderline and/or the TOE method shows that the unknowns are a significant portion of the emission profile, the permitting authority may decide to do any or all of the following:

1. Describe in a narrative form what is known of the unknown portion of the emissions.

2. Attribute a risk to the unknown portion of the emissions. An example was presented as a preferred option in U.S. EPA (1994d) which assumed that the unknown compounds are similar in toxicity and chemical properties to the known compounds taken as a whole. The referenced equation is as follows:

$$Q_{i,adj} = Q_i \cdot \frac{TO_{TOTAL}}{\sum_i C_i}$$ Equation 2-2A

where

$Q_{i,adj}$ = adjusted emission rate of compound *i* (g/s)
$Q_{i,}$ = emission rate of compound *i* (g/s)
TO_{TOTAL} = total organic emission (mg/m^3)
C_i = stack concentration of the *i*th identified COPC (mg/m^3)

3. Require additional testing to identify a greater fraction of the organic compounds.

4. Specify permit conditions that further control total organic emissions or that further control the risks associated with known emissions.

Permitting authorities may use variations of the TOE factor to address site-specific concerns. For example, some permitting authorities may compute three separate TOE factors based on the apportioning provided by the TOE test (i.e., TO_{VOC}, TO_{SVOC}, and TO_{GRAV}). The unknowns associated with each separate fraction of unidentified organic compounds can then be evaluated separately.

2.2.2 Estimating Emission Rates for Facilities with Multiple Stacks

Emissions from all combustion units burning hazardous waste at a facility, not just the unit currently undergoing the permitting process, should be considered in the risk assessment. As discussed further in Chapter 3, air dispersion modeling for each combustion unit (source) should be conducted separate from the other combustion units, to allow evaluation of risk on a stack or source-specific basis. A case example is where a chemical manufacturing facility may operate both an on-site incinerator and several hazardous waste burning boilers. Whether it is the incinerator or the boilers undergoing the permitting process, the risk assessment should consider the emissions from all the combustion units in the estimate of facility risk. In addition to RCRA combustion units, emissions from other RCRA treatment, storage, or disposal units (e.g., open burning/open detonation and thermal desorption) may also be included in the risk evaluation in some cases.

2.2.3 Estimating Stack Emission Rates for Facilities Not Yet Operational

New hazardous waste combustion facilities should submit a Part B permit application, go through an extensive permitting process, and, if successful, receive a final permit to commencement of operation. The permitting process requires submittal of sufficiently detailed information for the regulatory authorities to evaluate compliance with existing regulations, guidance, and protectiveness. Stack (source) locations and dimensions, design flow and emission rate estimates, waste feed characteristics, surrounding building dimension data, facility plot plans, and terrain data should be reviewed and used in a pre-operation risk assessment. This will assist in decision-making and designing permit requirements.

The design emission rates, waste feed characteristics, and other design data should be reviewed along with supplementing documentation to assure they are representative, accurate, and comprehensive. Good engineering practice dictates a check of, and comparison with, data from similar existing units. Stack test reports for facilities of similar technology, design, operation, capacity, auxiliary fuels, waste feed types, and APCSs should be used to estimate COPC emission rates for new facilities that have not been constructed.

If the preferred option of using surrogate data from similar facilities is not available, some state environmental agencies enforce emission rate limits based on state laws. Since these limits cannot be exceeded, they can be used to develop emission rate estimates for the risk assessment. The facility will demonstrate that its emissions are less than the those considered in the permit and risk assessment during the trial or risk burn.

Other data which may cause problems when performing risk assessments for new facilities is particle size distribution. A default particle size distribution is presented in Chapter 3 for use if particle size distribution data from a similar type of facility are not available.

2.2.4 Estimating Stack Emission Rates for Facilities Previously Operated

Emissions from the historical operation of combustion units burning hazardous waste at a facility, not just the unit currently undergoing the permitting process, may also be considered in the risk assessment on a

case-by-case basis as determined by the permitting authority. Such a case may be when the emissions from historical operation of a source or sources may have already resulted in potential risk concerns at or surrounding the facility. Emissions from historical operations could be taken into consideration by modeling as a separate source or, if applicable, in the fate and transport equations by adding the previous years of operation to the anticipated time period of combustion for a new or existing operating source. In addition to RCRA combustion units, historical emissions from other RCRA treatment, storage, or disposal units (e.g., open burning/open detonation and thermal desorption) at the facility under evaluation may also be included in the risk assessment in some cases.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- All stack test reports for combustion units used to develop emission rate estimates
- If using surrogate data for a new facility, descriptions of how the combustion data used represent similar technology, design, operation, capacity, auxiliary fuels, waste feed types, and APCSs
- Demonstration that the data used to develop the emission rate estimates were collected by using appropriate U.S. EPA sampling and analysis procedures
- The range of data obtained, and values used, in completing the risk assessment

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Facilities may use estimated emission rate data from other combustion units only to determine whether the construction of a new combustion unit should be completed. After a combustion unit has been constructed, U.S. EPA OSW will require an additional risk assessment using emission rates collected during actual trial burn conditions.

2.2.5 Emissions From Process Upsets

Uncombusted hazardous waste can be emitted through the stack as a result of various process upsets, such as start-ups, shutdowns, and malfunctions of the combustion unit or APCS. Emissions can also be caused by operating upsets in other areas of the facility (e.g., an upset in a reactor which vents gases to a boiler burning hazardous waste could trigger a process upset in the boiler, resulting in increased emissions). U.S.

EPA (1994d) indicates that upsets are not generally expected to significantly increase stack emissions over the lifetime of the facility.

Process upsets occur when the hazardous waste combustion unit is not being operated as intended, or during periods of startup or shutdown. Upset emissions are generally expected to be greater than stack emissions (over short periods of time) because the process upset results in incomplete destruction of the wastes or other physical or chemical conditions within the combustion system that promote the formation and/or release of hazardous compounds from combustion stacks. Upset emissions usually occur during events and times when the hazardous waste combustion unit is not operating within the limits specified in a permit or regulation.

To account for the increased emissions associated with process upsets, the stack emission rate estimated from trial burn data (upset factor is not applied to non-PIC emission rate estimates where the total mass of a constituent in the waste feed is assumed to be emitted) is multiplied by an upset factor. When available, facilities should use site specific emissions or process data to estimate the upset factor. The following types of data may be considered and evaluated to derive the upset factor:

- Data for continuous emissions monitoring systems that measure stack carbon monoxide, oxygen, total hydrocarbon (if required), or opacity (if appropriate)
- Data on combustion chamber, APCS, or stack gas temperature
- Frequency and causes of automatic waste feed cutoffs (AWFCO)
- Ratio of AWFCO frequency and duration to operating time
- APCS operating variables, such as baghouse pressure drop, liquid scrubber flow rate, or electrostatic precipitator voltage
- Stack test collected while the combustion unit was operated under upset conditions

This information may be analyzed with the objective of estimating the magnitude of the increase in emissions and the percentage of time on an annual basis that the unit operates at upset conditions.

When site specific data are not available or are inappropriate for deriving an upset factor, consistent with previous guidance (U.S. EPA 1993h), U.S. EPA OSW recommends that upset emissions be estimated by using a procedure based on work by the California Air Resources Board (CARB) (1990).

> ***Estimating Emissions from Process Upsets:*** To represent stack emission rates during process upsets, multiply the emission rate developed from the trial burn data by 2.8 for organics and 1.45 for metals. These factors are derived by assuming that emissions during process upsets are 10 times greater than emissions measured during the trial burn. Since the unit does not operate under upset conditions continually, the factor must be adjusted to account for only the period of time, on an annual basis, that the units operates under upset conditions. For organic compounds, the facility is assumed to operate as measured during the trial burn 80 percent of the year and operate under upset conditions 20 percent of the year [(0.80)(1)+(0.20)(10)=2.8]. For metals, the combustion unit is assumed to operate as measured during the trial burn 95 percent of the year and operate under upset conditions the remaining 5 percent of the year [(0.95)(1)+(0.05)(10)=1.45].

Catastrophic process upsets brought about by complete failure of combustion and air pollution control systems resulting from non-routine events such as explosions, fires, and power failures are considered accidental releases and are not addressed by this guidance.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Historical operating data demonstrating the frequency and duration of process upsets
- A discussion on the potential cause of the process upsets
- Estimates of upset magnitude or emissions
- Calculations which describe the derivation of the upset factor.

2.2.6 RCRA Fugitive Emissions

RCRA fugitive emission sources that should be evaluated in the risk assessment include waste storage tanks; process equipment ancillary to the combustion unit; and the handling and disposal of combustion system residues such as ash. Fugitive emissions from other RCRA treatment, storage, or disposal units (e.g., landfills) may also require evaluation in some cases.

This section contains guidance for quantitatively estimating fugitive emissions on the basis of procedures outlined by other U.S. EPA guidance. Guidance regarding air dispersion modeling of fugitive emissions is presented in Chapter 3.

2.2.6.1 Quantitative Estimation of RCRA Fugitive Emissions from Process Equipment

Quantitative estimation of RCRA fugitive emissions includes (1) identifying equipment to be evaluated as fugitive emission source(s), (2) grouping equipment, as appropriate, into a combined source, and (3) estimating compound specific emission rates for each source. Figure 2-1 is an example of a facility plot plan that includes one RCRA combustion unit (CU-1), two hazardous waste feed storage tanks (WST-1 and WST-2), and ancillary equipment identified in a RCRA Part B permit application for a hypothetical example facility. This figure, as well as Tables 2-1 and 2-2, have been provided as an example to facilitate understanding of each of the steps presented for estimating fugitive emissions.

Step 1: Identifying Fugitive Emission Sources - Generally, RCRA fugitive emission sources to be evaluated in the risk assessment should include waste storage tanks and process equipment that comes in contact with a RCRA hazardous waste such as equipment specified in Title 40, Code of Federal Regulations (40 CFR) Part 265, Subpart BB. Equipment covered under Subpart BB includes the following:

TABLE 2-1
EXAMPLE CALCULATION
TOTAL FUGITIVE EMISSION RATES
FOR EQUIPMENT IN WASTE FEED STORAGE AREA

1	2	3	4	5	6		7	8	9	10
Fugitive Emission Source	**Waste Stream**	**Type of Waste Stream In Service**	**Equipment Type**	**Number of Each Equipment Type Per Waste Stream**	**Equipment Emission Factors**		**Total VOC Weight Fraction**	**Operational Time Period of Equipment (days)**	**Total VOC Emissions Rate by Equipment (g/sec)**	**Total Fugitive Emission Rate (g/sec)**
					(kg/hr)	**(g/sec)**				
Waste Feed Storage Area	Process A Wastes	Light Liquid	Pumps	3	0.01990	0.00553	0.9	180	0.01493	0.14926
		Light Liquid	Valves	70	0.00403	0.00112	0.9	180	0.07056	
		Light Liquid	Connectors	30	0.00183	0.00051	0.9	180	0.01377	
		Light Liquid	Tank WST-1	1	--	--	0.9	180	0.02	
		Light Liquid	Tank WST-2	1	--	--	0.9	180	0.03	
	Process B Wastes	Heavy Liquid	Pumps	2	0.00862	0.00239	0.6	180	0.00287	0.06857
		Heavy Liquid	Valves	75	0.00023	0.00112	0.6	180	0.0504	
		Heavy Liquid	Connector	50	0.00183	0.00051	0.6	180	0.0153	
		Heavy Liquid	Tank WST-1	1	--	--	0.6	0	0	
		Heavy Liquid	Tank WST-2	1	--	--	0.6	0	0	

Notes:

Column 1	Equipment in the Waste Feed Storage Area was identified and grouped as a combined RCRA fugitive emission source with an area extent defined by UTM coordinates (NAD83).
Column 2	The waste streams serviced by equipment in the Waste Feed Storage Area can be determined through review of the facility's RCRA Part B Permit Application, Air Emission Standards.
Column 3	The type of waste stream in service, defined as light or heavy for determination of equipment specific emission factors, can be determined from review of waste stream vapor pressure.
Column 4	Similar types of equipment can be grouped according to the most applicable equipment specific emission factor and type of waste stream service (light or heavy) provided in U.S. EPA (1995f).
Column 5	The number of equipment per type at the source was multiplied by the equipment specific emission factor (Column 6) to obtain equipment specific emission rate for that respective type of equipment (Column 7).
Column 6	Emission factors specific to each type of equipment can be obtained from U.S. EPA (1995f), with the exception of storage tanks.
Column 7	Weight fraction of total volatile organic compounds was obtained from dividing the concentration of VOCs (mg/L) by the density of the waste stream (mg/L).
Column 8	Assumed the equipment is operational for 180 days a year.
Column 9	Equipment specific fugitive emission rates were determined by multiplying Columns 5, 6, and 7. Emission rates for tanks were obtained from Title V air permit application. In the absence of such data, emission rates for tanks can be calculated using U.S. EPA's TANKS Program or by following the procedures outlined in U.S. EPA (1995a).
Column 10	The total fugitive emission rate for each waste stream is determined by summing emission rates for all the equipment. Table 2-2 presents calculations for estimating speciated fugitive emissions.

TABLE 2-2

EXAMPLE CALCULATION
SPECIATED FUGITIVE EMISSIONS
FOR EQUIPMENT IN WASTE FEED STORAGE AREA

1	2	3	4	5	6
Fugitive Emission Source	**Waste Stream**	**Waste Stream Composition**	**Weight Fraction of Each VOC In Waste Stream (%)**	**Total Fugitive Emission Rate (g/sec)**	**Speciated Fugitive Emissions (g/sec)**
Waste Feed Storage Area	Process A Wastes	Acetaldehyde	0.20	0.14926	0.0030
		Acetonitrile	0.25		0.0037
		2-Nitropropane	0.25		0.0037
		Nitromethane	0.20		0.0030
	Process B Wastes	Acetaldehyde	0.20	0.06857	0.0137
		Acetonitrile	0.10		0.0069
		Methanol	0.20		0.0137
		Propionitrile	0.05		0.0034

Notes:

Column 1 Equipment in the Waste Feed Storage Area was identified and grouped as a combined RCRA fugitive emission source with an aerial extent defined by UTM coordinates (NAD83).

Column 2 The waste streams serviced by equipment in the Waste Feed Storage Area can be determined through review of the facility's RCRA Part B Permit Application, Air Emission Standards.

Column 3 The waste stream composition can be determined from analytical data

Column 4 Weight fraction of compounds in the waste stream can be determined from analytical data or review of the facility's Title V Air Permit Application, Emissions Inventory Questionnaire (EIQ) for Air Pollutants (see example in Figure 2-2).

Column 5 The total fugitive emission rate for each waste stream was obtained from Column 10, Table 2-1.

Column 6 Speciated fugitive emissions were obtained by multiplying Column 4 and 5.

- Pumps
- Valves
- Connectors (flanges, unions, tees, etc.)
- Compressors
- Pressure-relief devices
- Open-ended lines
- Product accumulator vessels
- Sampling connecting systems
- Closed vent systems
- Agitators

Each fugitive emission source should be identified on a facility plot map with a descriptor and the location denoted with Universal Transverse Mercator (UTM) coordinates (specify if North American Datum [NAD] of 27 or NAD83).

Step 2: Grouping Equipment Into a Combined Source - To significantly reduce the effort required to complete air dispersion modeling and subsequent risk assessment, equipment in close proximity may be grouped and evaluated as a single combined source with the speciated emission rates for each piece of equipment summed. The area extent of the grouped or combined source, as defined by UTM coordinates (specify if NAD27 or NAD83), should be clearly denoted on a facility plot map. The area extent of the combined source should be defined by the actual locations of the equipment being grouped, without exaggeration to cover areas without fugitive sources. Consideration should also be made for how fugitive emission sources are to be defined when conducting the air dispersion modeling (see Chapter 3).

As shown in Figure 2-1, equipment in two areas at the hypothetical facility have been grouped into combined sources; these consist of the Waste Feed Storage Area and the RCRA Combustion Unit Area.

Step 3: Estimating Fugitive Emissions from Tanks - Fugitive emission rates for waste storage tanks can be obtained from the facility's emission inventory or Title V air permit application prepared in compliance with Clean Air Act Amendments of 1990 (see example provided as Figure 2-2). If the facility does not have such information available, fugitive emissions from storage tanks can be calculated using U.S. EPA's TANKS Program or by following the procedures outlined in U.S. EPA guidance document (1995a), *"Compilation of Air Pollution Emission Factors, January 1995."*

FIGURE 2-1
EXAMPLE FACILITY PLOT MAP

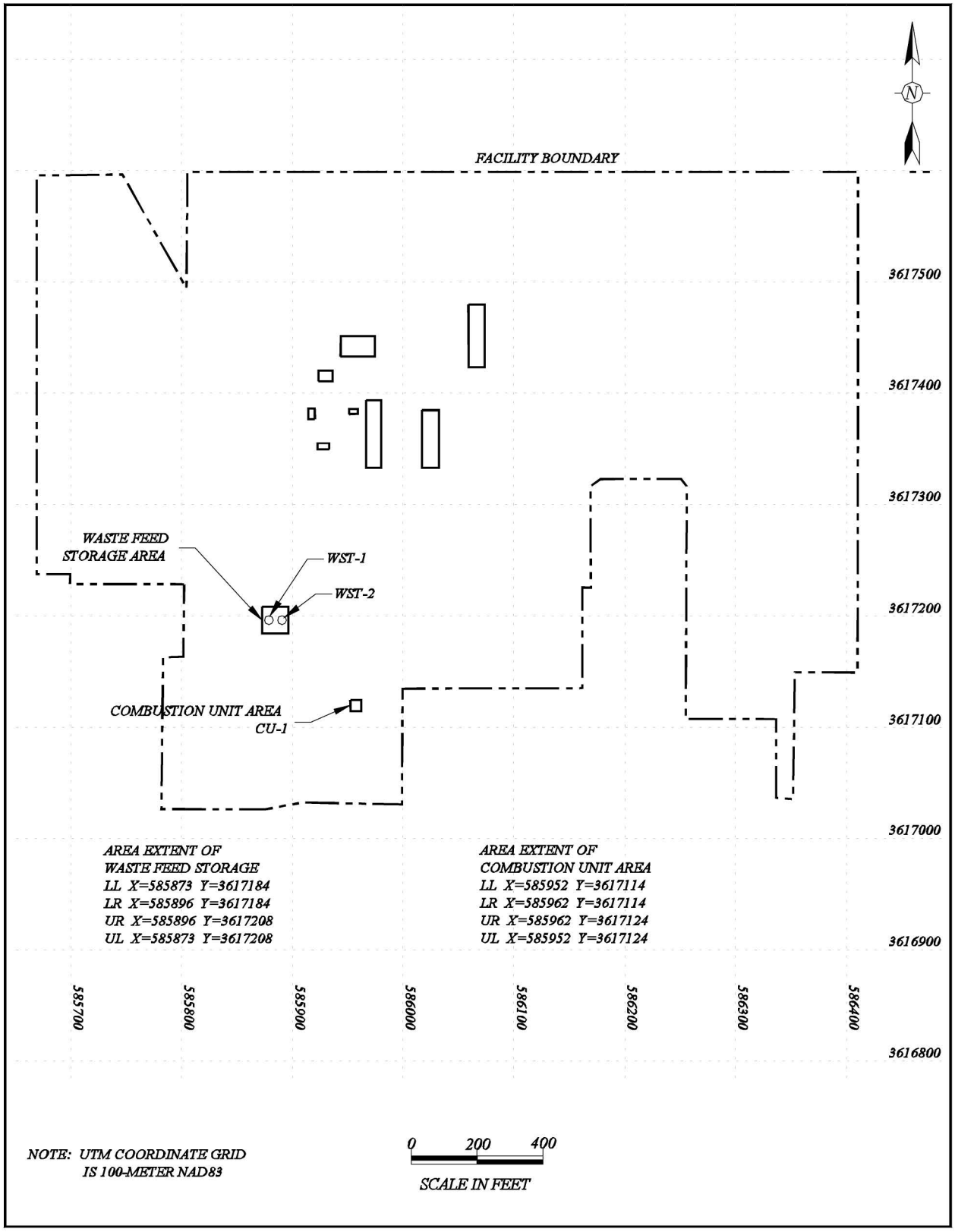


FIGURE 2-2
EXAMPLE EMISSIONS INVENTORY

Department of Environmental Quality *Air Quality Division* *P. O. Box 82135* *Baton Rouge, LA 70884-2135* *(504) 765-0219*	***LOUISIANA*** ***SINGLE POINT SOURCE / AREA SOURCE*** ***Emission Inventory Questionnaire (EIQ)*** ***for Air Pollutants***	*LA DEQ*

Company Name	*Plant location and name (if any)*	*Date of submittal*
Hypothetical Chemical Company	*Baton Rouge, LA Plant*	*February 1996*

Source ID Number	*Descriptive name of the equipment served by this stack or vent*	*Location of stack or vent (see instructions on how to determine location of area sources)*
WST - 1	*Waste Feed Tank*	*UTM zone no. 15* *Horizontal Coordinate 589100 m E* *Vertical coordinate 3616200 m N*

STACK and DISCHARGE PHYSICAL CHARACTERISTICS	***Height of stack above grade [ft]***	***Diameter or stack discharge area***	***Stack gas exit temperature (°F)***	***Stack gas flow at process conditions, not at standard (cfm)***	***Stack gas exit velocity (ft/sec)***	***For tanks, list volume (gals)***
Change [ ] yes [x] no	***8***	***0.167 ft***	***125***	***24.27***	***18.32***	***800*** ***Date of construction***

Fuel	***Type of fuel used and heat input (see instructions)***		*Operating Characteristics*	*Percent of annual throughout of pollutants through this emission point*				*Normal operating time of this point*			*Normal operating rate*
	Type of Fuel	***Heat input (MMBtu/hr)***		***Dec-Feb***	***Mar-May***	***Jun-Aug***	***Sep-Nov***	*hrs/ day*	*days/ week*	*weeks/ year*	
a				***25***	***25***	***25***	***25***	*24.00*	*7*	*52.0*	*100%*
b											
c											

Air Pollutant Specific Information

Pollutant	***Control equipment code***	***Control equipment efficiency***	***Emission Rate***			***Emission estimation method***	***Add, change, delete code***	***Concentration in gases exiting at stack***
			Average (lbs/hr)	***Maximum (lbs/hr)***	***Annual (tons/yr)***			
2-Nitropropane	***000***	***0.0000***	***0.0023***	***0.3463***	***0.01***	***3***	***c***	***N/A ppm by vol***
Acetaldehyde	***000***	***0.0000***	***0.0041***	***125.00***	***0.081***	***3***	***c***	***N/A ppm by vol***
Acetanitrite	***000***	***0.0000***	***0.0023***	***21.1266***	***0.01***	***3***	***c***	***N/A ppm by vol***
Methanol	***000***	***0.0000***	***0.0023***	***4.502***	***0.01***	***3***	***c***	***N/A ppm by vol***
Non-Toxic Voc	***000***	***0.0000***	***0.0062***	***195.3347***	***0.028***	***3***	***c***	***N/A ppm by vol***

The information required for estimating fugitive emission rates from storage tanks includes, but is not limited to, the following:

- Dimensions of the tanks
  - Shell height and diameter
- Characteristics of the tank roof
  - Color and shade
  - Condition (e.g., poor, good)
  - Type (e.g., cone, dome)
  - Height
  - Radius or slope
  - Fixed or floating
- Characteristics of the shell
  - Color and shade
  - Condition (e.g., poor, good)
  - Heated
- Settings on breathe vents
  - Vacuum setting
  - Pressure setting
- Characteristics of the stored liquids
  - Maximum and annual average liquid height
  - Working volume
  - Turnovers per year
  - Net throughput
  - Average annual temperature
  - Vapor pressures of speciated constituents (at annual average temperature)

Step 4: Estimating Fugitive Emissions from Process Equipment - Based on guidelines provided in U.S. EPA (1995f), *"Protocol for Equipment Leak Emission Estimates, EPA-453/R-93-017,"* fugitive emissions for each equipment listed under 40 CFR Part 265, Subpart BB can be estimated by the following four approaches, in order of increasing refinement and data requirements:

- Average Emission Factor Approach (AEFA)
- Screening Ranges Approach (SRA)
- U.S. EPA Correlation Approach (EPACA)
- Unit-Specific Correlation Approach (USCA)

These four approaches can be used at any facility to estimate fugitive emission rates of volatile organic compounds (VOCs) from equipment. Except for the AEFA method, all of the approaches require screening data collected by using a portable monitoring device (PMD). Because data on fugitive emissions at a facility is generally limited, the AEFA method will apply in most cases, and therefore, has been selected for use in the example demonstrated in Figure 2-1, and Tables 2-1 and 2-2. However, U.S. EPA OSW recommends that facilities use more refined approaches such as SRA, EPACA, or USCA, if sufficient data is available. U.S. EPA (1995f) provides a detailed discussion on these three approaches.

An Example Calculation Using the AEFA Method

Information for estimating fugitive emission rates using the AEFA method is as follows:

- Type of waste stream associated with each equipment type (Columns 2 and 3, Table 2-1)
  - light liquids are those in which the sum of the concentration of individual constituents with a vapor pressure over 0.3 kilopascals (kPa) at 20°C is greater than or equal to 20 weight percent
  - heavy liquids are all others liquids not meeting the definition of light liquids as specified above
- Number of each equipment type associated with each waste stream (Columns 4 and 5, Table 2-1)
- Total VOC weight fraction of each waste stream (Column 7, Table 2-1)
- Weight fraction of each VOC in each waste stream (Columns 3 and 4, Table 2-2)
- Operational time period of equipment (Column 8, Table 2-1)

When this approach is used, equipment can be grouped by waste streams of similar characteristics and VOC composition (Columns 1 and 2, Table 2-1). However, the AEFA approach does not account for different site-specific conditions such as temperature, vapor pressure, or screening values, among process units within a source category. Site-specific factors can significantly influence fugitive emission rates of leaks from equipment.

The average emission factors for synthetic organic chemicals manufacturing industry process units, refineries, and natural gas plants are presented in U.S. EPA (1995f) (Column 6, Table 2-1). The following

table is an excerpt from this guidance document. These emission factors are most valid for estimating rates of emissions from a grouping of equipment over a long time period.

SOCMI AVERAGE EMISSION FACTORS		
Equipment type	**Service**	**Emission factor (kg/hr/source)**
Valves	Gas Light liquid Heavy liquid	0.00597 0.00403 0.00023
Pump seals	Light liquid Heavy liquid	0.0199 0.00862
Compressor seals	Gas	0.228
Pressure relief valves	Gas	0.104
Connectors	All	0.00183
Open-ended lines	All	0.0017
Sampling connectors	All	0.0150

Source: U.S. EPA (1993e)

The total VOC emissions rate for a specified equipment type can be calculated by multiplying the equipment emission factor by the total VOC weight fraction and the number of each equipment type per waste stream (Column 9, Table 2-1 = Column 6 x Column 7 x Column 5).

The total VOC emission rates for each equipment type are summed to generate the total fugitive emission rate for the waste stream by (Column 10, Table 2-1). Speciated fugitive emissions can then be calculated by multiplying the weight fraction of each VOC in the waste stream and the total fugitive emission rate for the waste stream (Column 6, Table 2-2 = Column 4 x Column 5). This speciated emission rate is the emission rate used in the risk assessment.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Summary of the step-by-step process conducted to evaluate fugitive emissions
- Facility plot map clearly identifying each fugitive emission source with a descriptor and the location denoted with UTM coordinates (specify if NAD27 or NAD83).
- Speciated emission rate estimates for each waste stream serviced by each source, with supporting documentation
- Applicable discussion of monitoring and control measures used to mitigate fugitive emissions

2.2.6.2 Fugitive Emissions from Combustion Unit Leaks

Fugitive emissions that result from the construction, design, or operation of a combustion unit burning hazardous waste should be evaluated, as appropriate. Examples of fugitive emissions from combustion unit leaks include the following:

- Combustion units that operate under negative pressure may experience temporary positive pressures ("puffing") that cause fugitive emissions. This condition can occur when a slug of high BTU waste is combusted, causing a rapid expansion in the volume of combustion gases that exceeds the volume of the combustion chamber.
- Fugitive emissions resulting from the day-to-day operation of the combustion unit and APCS. These emissions will typically include (1) leaks that occur due to a positive pressure in the APCS, and (2) routine maintenance activities such as replacement of baghouse collection bags.

Currently, U.S. EPA OSW does not offer any specific quantitative guidance on how to estimate fugitive emissions from hazardous waste combustion units. However, risks associated with emissions from hazardous waste combustion unit leaks can be addressed in the uncertainty section of the risk assessment if no site specific quantitative methods are available. Specifically, the permitting authority can review facility specific data to determine whether or not the design addresses equipment leaks and whether the operational data indicates that equipment leaks may be a problem.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Process design information and drawings (if necessary)
- Past operating data indicating the frequency, duration, and magnitude of combustion unit leaks
- Information regarding the probable cause of combustion unit leaks
- Summary of procedures in place to monitor or minimize fugitive emissions resulting from combustion unit leaks

2.2.7 RCRA Fugitive Ash Emissions

The combustion of hazardous waste materials may result in the production of flyash. Fugitive particle emissions may result from the subsequent collection, handling, and disposal of the flyash. Typically, fugitive emissions of flyash, collected from an air pollution control device (APCD) will occur during transfer into covered trucks or other conveyance mechanisms prior to disposal. Emissions generated during the loading process can be controlled by APCDs or other types equipment, however, a fraction of the flyash may still escape into the atmosphere as fugitive emissions.

2.2.7.1 Quantitative Estimation of RCRA Fugitive Ash Emissions

Steps for the quantitative estimation of RCRA fugitive ash emissions include (1) determining an empirical emission factor, (2) estimating the flyash generation rate, and (3) accounting for air pollution control equipment, if applicable. As demonstrated in the example calculation below, the fugitive ash emission rate can then be estimated by multiplying the empirical emission factor by the flyash generation rate and the control deficiency of the air pollution control equipment, if applicable.

Step 1: Determining an Empirical Emission Factor - Particle emissions associated with flyash loading and unloading can be estimated using an empirical emission factor of 1.07 lb per ton flyash. This factor is based on a field testing program conducted at a coal fired power plant equipped with an electrostatic precipitator (ESP) (Muleski and Pendleton 1986). Because the combustion of coal and hazardous wastes are similar activities, flyash generated from similar control devices is expected to behave similarly under the same conditions, with respect to fugitive emissions. In general, particle behavior is dependent more on the physical form of the flyash than on the feed (or waste) stream being combusted. The emission factor determined during the empirical study (0.107 lb per ton flyash) can be adjusted by a factor (e.g., 10) to account for the fact that the flyash

from the combustion of coal (as in the study) was wetted. Flyash from the hazardous waste combustion facility may not be wetted depending on the facility.

Step 2: Estimating the Flyash Generation Rate - The flyash generation rate from the APCD can be obtained from the Part B Permit Application and the total ash content of the "generic" waste streams created from the waste profile. Both values should be approximately the same. Since a major portion of ash fed to the combustor is converted to bottom ash, it is likely that this value is a conservatively high estimate of the actual flyash generation rate.

Step 3: Accounting for Air Pollution Control Equipment - If an APCD is used for controlling emissions during flyash handling operations, an efficiency factor (e.g., 99.5 percent) can be applied to the emission rate. An efficiency factor of 99.5 percent is based on U.S. EPA (1995a) for typical collection efficiencies of particulate matter control devices, for the particle sizes in the range of 2.5 to 10 um.

Example Calculation

The fugitive ash emission rate is calculated by multiplying the empirical emission factor (Step 1) times the estimated flyash generation rate (Step 2) [(1.07 lb per ton) * (5,000 tons per year) = 5,350 lbs per year]. Accounting for the air pollution control equipment, the product of Steps 1 and 2 is multiplied times one minus the fabric filter efficiency (Step 3) to obtain the final RCRA fugitive ash emission rate for use in the risk assessment [(5,350 lbs per year) * (1 - 0.995) = 26.75 lbs per year].

2.2.8 Cement Kiln Dust (CKD) Fugitive Emissions

CKD is the particulate matter (PM) that is removed from combustion gas leaving a cement kiln. This PM is typically collected by an APCS—such as a cyclone, baghouse, ESP—or a combination of APCSs. Many facilities recycle a part of the CKD back into the kiln. Current and applicable guidance on evaluating CKD includes (1) the *Technical Background Document for the Report to Congress* (U.S. EPA 1993g), and (2) the more recent regulatory determination of CKD (60 FR 7366, February 7, 1995).

Most CKD constituents (for example, metals) are not volatile but could be released to air through fugitive dust emissions as a volatile or semivolatile organic that can be released in gaseous form and present in relatively low concentrations, if at all (U.S. EPA 1993a). Dust particles may be suspended in the air by either wind erosion or mechanical disturbances. The extent to which dust is blown into the air by wind erosion depends on several site-specific characteristics, including (1) the texture (particle size distribution)

and moisture content of the CKD on the surface of piles, (2) nonerodible elements, such as clumps of grass or stones on the pile, (3) a surface crust, and (4) wind speeds. Mechanical disturbances that can suspend CKD constituents in the air include (1) vehicular traffic on and around CKD piles, (2) CKD dumping and loading operations, and (3) transportation of CKD around a plant site in uncovered trucks. Cement plants may use various control measures to limit the release of CKD to the air. For example, CKD may be pelletized in a pug mill, compacted, wetted, and covered to make the material less susceptible to wind erosion.

To keep the dust down, many facilities add water to CKD, before disposal, to agglomerate individual particles. In addition, as CKD sits in a pile exposed to the elements, occasional wetting by rainfall may form a thin surface crust in inactive areas of the pile. This acts to mitigate air entrainment of particles. However, based on field observations by U.S. EPA (1993g), neither surface wetting nor natural surface crusting eliminates the potential for CKD to be blown into the air. Wetting the dust before disposal provides incomplete and temporary control, because (1) infrequent application of water, and (2) the dust ultimately dries and returns to a fine particulate that is available for suspension and transport. Similarly, a surface crust may develop, but (1) the crust breaks when vehicles or people move on the pile, and (2) fresh dust is regularly added to the pile, providing a continual, exposed reservoir of fine particles. It should be noted that a crust does not always form for a variety of reasons such as weather and chemistry of the CKD.

CKD constituents that are released to the air are transported and dispersed by the winds, and are ultimately deposited onto land or water, either by settling in a dry form or by being entrained in precipitation.

2.2.8.1 Composition and Characteristics of CKD

U.S. EPA (1993g) highlighted the limited amount of available information regarding the variation in chemical constituents of CKD generated by facilities burning hazardous waste as fuel and by facilities burning only fossil or nonhazardous waste fuels. There may also be differences in composition between the "as-generated" CKD that is recycled back into the system and the "as-managed" CKD that is disposed on or offsite.

Transport in air is of concern for CKD, because the dust is a fine PM that is readily suspendable, transportable, and respirable in air. In general, particles that are $\leq$100 micrometers may be suspended in

the wind and transported. Within this range, particles that are ≤30 micrometers can be transported for considerable distances downwind. Virtually all of the dust generated at the 15 facilities evaluated by U.S. EPA (1993g) in the *Cement Kiln Dust Report to Congress* may be suspended and transported in the wind (that is, the vast majority of particles are ≤100 micrometers), and over two-thirds of all CKD particles generated may be transported over long distances. Additionally, a significant percentage of the total dust generated (from 22 to 95 percent, depending on kiln type) comprises particles that are ≤10 micrometers.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Physical data, including particle size distribution and density
- Chemical data, including organic and inorganic analytical tests similar to those used for sampling combustion gases
- Plant net CKD generation rate (how much CKD per year that is available for disposal)
- Ambient air monitoring data
- CKD management, transportation, storage, and disposal methods
- Containment procedures, including fugitive dust prevention measures and the area of exposed CKD
- Meteorological data, including wind speed and precipitation

2.2.8.2 Estimation of CKD Fugitive Emissions

In general, this guidance does not address CKD risks in a quantitative fashion. However, risk assessments conducted for cement manufacturing facilities should, at a minimum, evaluate the fugitive emissions due to CKD on a qualitative basis. Readers are referred to the *Technical Background Document for the Report to Congress* (U.S. EPA 1993g), for methods to estimate the magnitude of fugitive emissions from the handling, storage, and disposal of CKD. In addition, an analysis of a specific facility's compliance with other environmental statutes and regulations may be an appropriate method to qualitatively evaluate risks associated the handling, storage, and disposal of CKD.

2.3 IDENTIFYING COMPOUNDS OF POTENTIAL CONCERN

Compounds of potential concern (COPCs) are those compounds evaluated throughout the risk assessment. The purposes of identifying COPCs are to focus the risk assessment on those compounds that are likely to pose the most risk to ecological receptors exposed to hazardous waste combustion emissions. The COPC identification process is conservative by design to avoid not including compounds that might pose an ecological risk.

There is no one definition of a COPC, because a compound that is a COPC at one hazardous waste combustion unit may not be a COPC at another combustion unit. COPCs in the emissions from hazardous waste combustion units vary widely, depending on (1) the type of combustion unit, (2) the type of hazardous waste feed being burned, and (3) the type of APCS used. Also considered as COPCs are products of incomplete combustion (PICs); which are any organic compounds emitted from a stack, such as (1) compounds initially present in the hazardous waste feed stream and not completely destroyed in the combustion process, and (2) compounds that are formed during the combustion process. Because PICs may be formed by trace toxic organic compounds in the waste feed stream, these compounds should be evaluated as PIC precursors, in addition to those compounds that constitute most of the hazardous waste feed.

PICs should not be confused with principal organic hazardous constituents (POHC), which are compounds in the waste feed stream used to measure DRE of the combustion unit during a trial burn test. Unburned POHCs and partially destroyed or reacted POHCs are PICs, but PICs are not necessarily related to POHCs.

Table A-1 (Appendix A) presents a comprehensive list of compounds typically identified (1) in hazardous waste, and (2) in hazardous waste combustion stack gas emissions. For each compound, Table A-1 identifies the Chemical Abstracts Service (CAS) number and also indicates whether a compound has been identified as a potential COPC by (1) U.S. EPA and state risk assessment reference documents, (2) emission test results that have identified the compound in the emissions from hazardous waste combustion facilities, or (3) other literature that suggests that the compound may be significant from a risk perspecitve. Table A-1 has been provided in this guidance in order to help risk assessors ensure that the trial burn considers the full range of compounds potentially emitted from a combustion unit and the

appropriate analytical method. Once the trial burn stack tests are completed, the COPC selection process is initiated based on the universe of stack test data, not Table A-1. The purpose of a risk assessment is not to arbitrarily evaluate every potential compound listed in Table A-1.

Based on U.S. EPA OSW review, COPCs previously identified in ecological isk assessments at combustion facilities are as follows:

- Polychlorinated dibenzo(p)dioxins (PCDD) and polychlorinated dibenzofurans (PCDF)
- Polynuclear aromatic hydrocarbons (PAH)
- Polychlorinated biphenyls (PCB)
- Pesticides
- Nitroaromatics
- Phthalates
- Other organics
- Metals

This list was compiled based on professional experience and is not meant to be either limiting or inclusive. The list enabled U.S. EPA OSW to focus on (1) developing receptor-specific and compound-specific biocentration factors as provided in Appendicies C and D, (2) developing compound- and receptor-specific *TRV*s as provided in Appendix E, and (3) developing receptor exposure parameters and exposure equations discussed in Chapter 5 and provided in Appendix F. These focused compound-specific parameters and information are included to facilitate the performance of ecological risk assessments, and are not meant to be either limiting or inclusive for hazardous waste combustion facilities. Experience has shown that developing compound-specific and receptor-specific parameters for risk assessments can be one of the most labor- and time-intensive parts of completing the risk assessment, and U.S. EPA OSW intends that the information included in the Appendicies of this guidance facilitates the risk process.

COPCs are identified from the trial burn data based on their potential to pose an increased risk. This identification process should focus on compounds that (1) are likely to be emitted, based on the potential presence of the compound or its precursors in the waste feed, (2) are potentially toxic to ecological

receptors, and/or (3) have a definite propensity for bioconcentrating in ecological receptors and bioaccumulating in food chains. Appendix E presents toxicity reference values of specific compounds to specific receptors. The toxicity information provided in this guidance is for informational purposes to help permitting authorities explain the basis for identifying compounds as COPCs and facilitate completing the risk assessment. Since toxicity information may change as additional research is conducted, permitting authorities should review the most current available information before completing a risk assessment to ensure that the toxicity data used in the risk assessment is based upon the most current Agency consensus.

As illustrated in Figure 2-3, the following steps should be used to identify the COPCs that will be evaluated for each facility (U.S. EPA 1993h; 1994d).

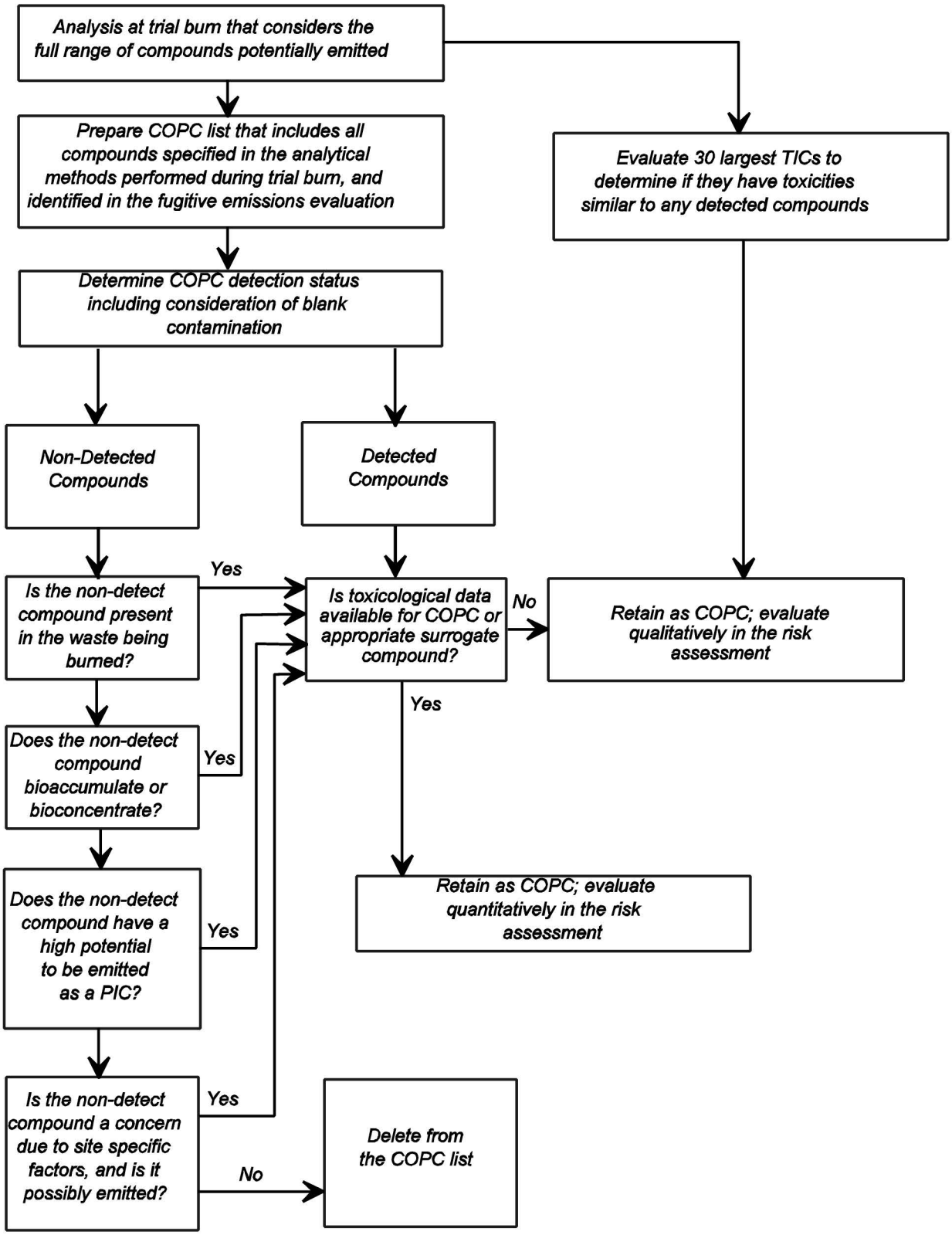
Step 1: Evaluate analytical data from the stack tests performed during the trial burn and compounds associated with fugitive emissions (see Section 2.2.5). Prepare a list which includes all the compounds specified in the analytical methods performed in the trial burn, and fugitive emission evaluation. Describe whether the compound was detected or not detected.

A detection in any one of the sample components (e.g., front half rinse, XAD resin, condensate, Tenax tube) in any run constitutes a detection for that specific compound. Evaluation of blank contamination results, included in the quality assurance (QA) data section of the trial burn report, should be considered when determining the non-detect status of the compounds (see Section 2.5).

Step 2: Evaluate the type of hazardous waste burned in the combustion unit—including all wastes that the unit will be permitted to burn—to determine whether any of the non-detect compounds should be retained for evaluation as COPCs because they are potentially present in the waste.

For example, if a facility is permitted to burn explosives which characteristically include nitroaromatic compounds, yet the stack test showed non-detect status for all nitroaromatic compounds, nitroaromatic compounds should still be evaluated in the risk assessment. This evaluation should also consider other materials fed to the combustion unit (e.g., raw materials or coal in a cement kiln). Regardless of the type of hazardous waste being burned in the combustion unit, every risk assessment should include PCDD/PCDFs and PAHs (the rationale for including these compounds is discussed in greater detail in Sections 2.3.1 and 2.3.2).

COPC IDENTIFICATION



Step 3: Include as COPCs those compounds that are non-detect, but have a high potential to be emitted as PICs.

Although some compounds (nitroaromatics, pthalates, hexachlorobenzene, and petachlorphenol) have traditionally been automatically identified as PICs in previous U.S. EPA guidance, inclusion of these compounds should be based on consideration of potential to be emitted and waste feed composition (e.g., nitrogenated wastes, plastics, or highly chlorinated organic waste streams) (see Sections 2.3.4 through 2.3.6).

Step 4: Include as COPCs those compounds that are non-detect, but have a tendancy to bioaccumulate or bioconcentrate. This includes organic chemicals with log K_{ow} values equal to or greater than 4.0 (Connolly and Pederson 1987), and inorganic compounds with a whole-body *BCF* equal to or greater than 100.

U.S. EPA OSW understands that this step would not retain some nondetected compounds (such as VOCs with log K_{ow} values less than 4.0) for further evaluation in the risk assessment and appears to provide the opportunity for detection limits for these compounds to be increased intentionally by the facility to escape the risk assessment process. However, U.S. EPA OSW anticipates that stack test data used in conducting the risk assessment will also be subject to evaluation in the human health risk assessment process, which would subsequently determine increased risk due to nondetected compounds with high detection limits. Therefore, the lowest achievable detection limits possible with standard U.S. EPA methods for all compounds are recommended, ensuring that the risk assessment process will result in the risk manager obtaining the information necessary to conclude that the facility has not potentially overlooked a serious risk.

Step 5: Evaluate the 30 largest tentatively identified compound (TIC) peaks obtained during gas chromatography (GC) analysis, to determine whether any of the TICs have toxicities similar to the detected compounds. If they do, consider surrogate toxicity data, as recommended for detected COPCs without toxicity information.

Step 6: Evaluate any compound that may be of concern due to other site-specific factors (e.g., community and regulatory concern, high background concentrations). Include as COPCs those compounds that (1) are a concern due to site-specific factors, and (2) may be emitted by the combustion unit.

If the compound in question does not have a reasonable potential of being present in the stack emissions, the risk assessment report should justify this assertion. This information will provide the risk manager with

the information necessary to evaluate potential for risk. By following Steps 1 through 6, the risk assessor will be able to identify COPCs from the typically exhaustive list of compounds tested in during the trial burn. To complete Step 4, log K_{ow} and *BCF* values for compounds typically identified in risk assessments as COPCs and listed at the beginning of this section are located in Appendicies A and C, respectively.

The following subsections also focus on compounds that can drive risk assessments as indicated by past experience. These compounds include polychlorinated dibenzo(p)dioxins and dibenzofurans, polynuclear aromatic hydrocarbons, polychlorinated biphenyls, nitroaromatics, phthalates, hexachlorobenzene and pentachlorophenol, and metals. Volatile organic compounds are also discussed. Specific issues that affect the COPC identification process and evaluation of these compounds in the risk assessment are discussed. Because U.S. EPA's boiler and industrial furnace (BIF) regulations also regulate emission rates of PM and hydrochloric acid and chlorine gas, the risks associated with these compounds are also discussed. There is also a discussion of the emerging issues surrounding the class of compounds called "endocrine disruptors."

U.S. EPA OSW recognizes that, for many compounds, only limited information is available regarding potential effects. In addition, for some compounds for which effects have been identified, the relationship between dose and response may be poorly understood. U.S. EPA OSW advocates that the risk assessment use the sum of the available toxicological information and evaluate the uncertainty associated with these issues. As stated previously, toxicity benchmarks and information may change as additional research is conducted, permitting authorities should consult with the most current information before completing a risk assessment. Toxicity profiles for many of the compounds typically evaluated in ecological risk assessments are presented in Appendix H. U.S. EPA OSW prepared these profiles to promote consistency in risk assessments and to assist the uncertainty analysis.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Complete evaluation of hazardous wastes to be burned in the combustion unit
- Complete evaluation of any raw materials or primary fuels burned in the combustion unit
- Waste analysis procedures used to monitor the composition of hazardous waste feed streams
- Analytical data and calculations used to complete the COPC identification process

2.3.1 Polychlorinated Dibenzo(p)dioxins and Dibenzofurans

Based on their combustion properties and toxicity, U.S. EPA OSW recommends that PCDDs and PCDFs should be included in every risk assessment. The general combustion properties and guidance for addressing toxicity of PCDDs and PCDFs are discussed in the following paragraphs and subsections, respectively.

One mode in which PCDDs and PCDFs form in dry APCSs is fly ash catalyzed reactions between halogens and undestroyed organic material from the furnace. PCDDs and PCDFs were first discovered as thermal decomposition products of polychlorinated compounds, including (1) the herbicide 2,4,5-T, (2) hexachlorophene, (3) PCBs, (4) pentachlorophenol, and (5) intermediate chemicals used to manufacture these compounds. In recent years, as chemical analytical methods have become more sensitive, additional sources of PCDDs and PCDFs have been identified, including (1) effluent from paper mills that use chlorine bleaches, and (2) combustion sources, including forest fires, municipal waste and medical incinerators, and hazardous waste combustion units. Duarte-Davidson et al. (1997) noted that the combustion of chlorine-containing materials in municipal solid waste is responsible for about two-thirds of the total annual emissions of newly formed TCDDs and TCDFs in the United Kingdom. In the United States, U.S. EPA (1998a) estimated that emissions of dioxin TEQs from municipal solid waste incinerators accounted for 37 percent of all emissions of dioxins into the environment in 1995.

PCDDs and PCDFs are formed at these combustion sources from the reaction of chlorine-containing chemicals and organic matter. Predicting the production of PCDDs and PCDFs in a specific situation is

difficult, because dechlorination, which produces PAHs from PCDDs and PCDFs, occurs under similar conditions. Recent studies (Addink et al. 1996; Environment Canada 1987; Fröese and Hutzinger 1996a, 1996b; Gullett et al.1994; Kilgroe et al. 1991; Luijk et al. 1994; Robert 1994) have explored some of these complexities, including (1) the formation of PCDDs and PCDFs from simple organics (such as ethane) and complex organics (such as dibenzofuran), and (2) the catalysis of these organic compound reactions by various common metals, such as copper. Wikström et al. (1996) found that the form of chlorine—whether organic, as with chlorinated solvents, or inorganic, as with bleach and salts—has little effect on the quantity of PCDDs and PCDFs formed. However, their study found that the total concentration of chlorine is important. In particular, if the waste being burned exceeds 1 percent chlorine, the PCDD and PCDF formation rate increases significantly. The formation rate of PCDDs and PCDFs may also depend on the physical characteristics of the waste feed stream. Solid waste streams or high-ash-content liquid waste feed streams may increase particulate levels in the combustion system between the combustion unit and the APCS. The increased particulate levels provide additional surfaces for catalysis reactions to occur.

A review of currently available dioxin data for combustion units reveals that total PCDD/PCDF emission rates vary by more than 28-fold between different facilities, even though they use similar combustion units and APCSs (U.S. EPA 1996h). Site-specific emission data are needed to enable completion of a more refined risk assessment at each combustion unit.

In evaluating fate-and-transport pathways, it is important to consider the chemical and physical properties of dioxins. In soil, sediment, and the water column, PCDDs and PCDFs are primarily associated with particulate and organic matter because of their high lipophilicity and low water solubility of the PCDDs and PCDFs. Evaluation of ambient air monitoring studies, in which researchers evaluated the partitioning of dioxin-like compounds between the vapor and particle phases, suggests that the higher chlorinated congeners (the hexa through hepta congeners) were principally sorbed to airborne particulates, whereas the tetra and penta congeners were significantly, if not predominantly, partitioned to the vapor phase (U.S. EPA 1994e). This finding is consistent with vapor/particle partitioning as theoretically modeled in Bidleman (1988). Dioxin-like compounds exhibit little potential for significant leaching or volatilization after they have been sorbed to particulate matter (U.S. EPA 1994e).

The guidance in Chapter 5 for modeling exposure to a COPC also applies generally to exposure assessment for PCDDs and PCDFs. However, procedures specific for these compounds should be followed because

congener-specific toxicity and bioaccumulation information is limited. As discussed below, exposure of receptors to PCDDs and PCDFs should be assessed using 2,3,7,8-TCDD toxicity equivalency factors (*TEF*) and 2,3,7,8-TCDD bioaccumulation equivalency factors (*BEF*) to convert the exposure media concentration of individual congeners to a 2,3,7,8-TCDD Toxicity Equivalent (TEQ).

U.S. EPA OSW is also aware of growing concern regarding the risks resulting from (1) fluorine- and bromine-substituted dioxins and furans, and (2) sulfur analogs of PCDDs and PCDFs. U.S. EPA guidance on considering these compounds as potential COPCs is discussed in Section 2.3.1.5.

2.3.1.1 Toxicity Equivalency Factors for PCDDs and PCDFs

There are 210 individual compounds or "congeners" of PCDDs and PCDFs. Evidence indicates that low levels of PCDD and PCDF congeners adversely affect ecological receptors, especially the 2,3,7,8-substituted congeners (U.S. EPA 1993p; Hodson et al. 1992; Walker and Peterson 1992). The 17 congeners containing chlorine substituents in at least the 2-, 3-, 7-, and 8-ring positions have been found to display dioxin-like toxicity (U.S. EPA 1993g; 1994h). Therefore, U.S. EPA OSW and other U.S. EPA guidance (1998; 1993h) recommend that all risk assessments include all PCDDs and PCDFs with chlorine molecules substituted in the 2, 3, 7, and 8 positions. In Appendix A, the 17 PCDD and PCDF congeners that should be evaluated in every risk assessment for potential risk are listed. Any other PCDD and PCDF congener identified as a COPC should be treated as an uncertainty (see Chapter 6).

As noted above, the toxicity of PCDDs and PCDFs is related to their structure and chlorine substitution pattern. The 17 listed congeners are known to share a common mechanism of toxicity involving binding to the Ah-receptor. Planar PCDDs and PCDFs are characteristic for high Ah-receptor affinity. Toxicity is also related to the chlorine substitution pattern, especially for chlorine atoms in the 2,3,7,8-positions. By extension, it is assumed that an additivity model may be used to characterize the toxicity of mixtures of these PCDDs and PCDFs. While these congeners share a similar toxicity mechanism, available information indicates that the toxicity of these PCDDs and PCDFs is congener-specific, resulting in a wide range of toxicities (U.S. EPA 1993p, World Health Organization [WHO] 1997). This has resulted in the development of TEFs for these 17 congeners to convert the exposure media concentration of individual congeners to a 2,3,7,8-TCDD TEQ; which are widely used to assess the risk of dioxin and dioxin-like compounds (U.S. EPA 1993p; WHO 1997).

The procedure used to assess risk on the basis of the relative toxicity of 2,3,7,8-TCDD, which is assumed the most toxic dioxin (U.S. EPA 1994f), assigns a TEF value to each congener relative to its toxicity in relation to 2,3,7,8-TCDD. For example, 2,3,7,8-TCDD has a TEF of 1.0, and the other PCDDs and PCDFs have TEF values between 0.0 and 1.0. To estimate the exposure media concentration, U.S. EPA OSW recommends that a risk assessment for PCDDs and PCDFs be completed using the congener-specific emission rates from the stack and fate and transport properties in the media concentration equations (see Chapter 3 and Appendix B) and food web equations (see Chapter 5 and Appendix F). For quantifying risk, the exposure media (e.g., may be sediment for evaluating risk to sediment community measurement receptors, or it may be the dose of one or more prey species for evaluating risk to class-specific guild measurement receptors) concentrations of the individual congeners should be converted to a 2,3,7,8-TCDD TEQ by multiplying by the congener-specific TEFs corresponding to the respective measurement receptor being evaluated. Use of the TEFs allows for the combined risk resulting from exposure to a mixture of the 17 dioxin-like congeners to be computed assuming that the risks are additive.

WHO (1997) recently convened a conference to discuss the derivation of TEFs for humans and wildlife. WHO (1997) discussed the compilation and review of relevant scientific information on the PCDD and PCDF toxicity to wildlife, and utilized this information to assist in identifying TEFs. The following table (see Table 2-3) lists congener-specific TEFs reported for fish, mammals, and birds (WHO 1997). U.S. EPA OSW believes that these conference proceedings reflect the best available information for screening the ecological risk of PCDDs and PCDFs. However, it should be noted that TEFs based on long term in-vivo studies should be used when available.

TABLE 2-3

POLYCHLORINATED DIBENZO-P-DIOXIN AND POLYCHLORINATED DIBENZOFURAN CONGENER TOXICITY EQUIVALENCY FACTORS (*TEF*s) FOR FISH, MAMMALS, AND BIRDS

Congener	Receptor		
	Fish TEF	Mammal TEF	Bird TEF
2,3,7,8-TCDD	1.0	1.0	1.0
1,2,3,7,8-PeCDD	1.0	1.0	1.0
1,2,3,4,7,8-HxCDD	0.5	0.1	0.05
1,2,3,6,7,8-HxCDD	0.01	0.1	0.01
1,2,3,7,8,9-HxCDD	0.01	0.1	0.1
1,2,3,4,6,7,8-HpCDD	0.001	0.01	<0.001[a]
OCDD	Not available	0.0001	Not available
2,3,7,8-TCDF	0.05	0.1	1.0
1,2,3,7,8-PeCDF	0.05	0.05	0.1
2,3,4,7,8-PeCDF	0.5	0.5	1.0
1,2,3,4,7,8-HxCDF	0.1	0.1	0.1
1,2,3,6,7,8-HxCDF	0.1	0.1	0.1
2,3,4,6,7,8-HxCDF	0.1	0.1	0.1
1,2,3,7,8,9-HxCDF	0.1	0.1	0.1
1,2,3,4,6,7,8-HpCDF	0.01	0.01	0.01
1,2,3,4,7,8,9-HpCDF	0.01	0.01	0.01
OCDF	0.0001	0.0001	0.0001

Notes:

[a] For exposure assessment, a value of 0.001, which estimates upper range of true value, should be used.

Toxicity Equivalency Factors for Fish

WHO (1997) reported the review of three scientific studies on the relative overt toxicity of PCDDs and PCDFs to fish from which TEFs could be determined. These included evaluation of rainbow trout sac fry mortality after egg injection (Walker and Peterson 1991; Zabel et al. 1995) and evaluation of rainbow trout sac fry mortality following waterborne exposure (Bol et al. 1989). WHO (1997) concluded that TEFs from the egg injection studies were more appropriate than the waterborne exposure study. WHO (1997)

also noted that since these TEFs were determined from the toxicity of each congener in relation to concentration in eggs, site-specific differences in exposure and bioavailability, and species-specific differences in toxicokinetic factors (deposition and metabolism) are accomodated. TEFs for PCDD and PCDF congeners in fish are presented in Table 2-3.

Toxicity Equivalency Factors for Mammals

Current TEFs for mammals (for evaluating human health risk to PCDDs and PCDFs) are largely based on studies in rodents. To supplement existing rodent-based TEFs, WHO (1997) discussed a mink reproductive study (Tillitt et al. 1996) and a study which analyzed available data from mink reproductive toxicity tests (Leonard et al. 1994). WHO (1997) reported that the relative potencies of PCDD and PCDF congeners toward mink reproductive toxicity were similar to the rodent models. WHO (1997) also discussed recent information on *in vivo* tumor promotion and in *vivo* ethoxyresorufin-o-deethylase (EROD) induction potency. However, specific studies reporting this information were not cited. Based on their review, WHO (1997) reported updated TEFs for mammals, including new values for 1,2,3,7,8-PeCDD, OCDD, and OCDF. TEFs for PCDD and PCDF congeners in mammals are presented in Table 2-3.

Toxicity Equivalency Factors for Birds

The experimental design of studies on the overt toxicity of PCDDs and PCDFs to birds precluded determination of the relative potency of these congeners. Other types of studies evaluated included embryo mortality following egg injection, *in vivo* biochemical effects following egg injection, biochemical effects in *in vitro* systems (Kennedy et al. 1996), and quantitative-structure activity relationship (QSAR) studies (Tysklind et al. 1995). The reviewed information indicated no significant differences between the *TEF* ranges for EROD induction and embryo mortality. Based on these results, WHO (1997) reported *TEF*s determined from EROD induction and QSAR studies. *TEF*s for PCDD and PCDF congeners in birds are presented in Table 2-3.

2.3.1.2 Exposure Assessment for Community Measurement Receptors

To evaluate exposure of water, sediment, and soil communities to PCDDs and PCDFs, congener-specific concentrations in the respective media to which the community is exposed should be converted to a

2,3,7,8-TCDD *TEQ*; which allows for direct comparison to 2,3,7,8-TCDD toxicity benchmarks. A media-secific 2,3,7,8-TCDD *TEQ* is calculated and used in the exposure assessment because limited congener-specific toxicity information is available for community receptors (WHO 1997). The congener-specific concentrations in the media to which the community being evaluated is exposed, should be calculated consistent with the guidance presented in Chapters 4 and 5, and Appendix F, for assessing exposure of community measurement receptors to other COPCs. The concentration of each PCDD and PCDF congener in the media of exposure should then be multiplied by the congener-specific *TEF* for fish (see Table 2-3), and summed, to obtain the 2,3,7,8-TCDD *TEQ* (see Equation 2-3).

$$TEQ = \sum (C_{Mi} \cdot TEF_i) \qquad \text{Equation 2-3}$$

where

TEQ	=	2,3,7,8-TCDD toxicity equivalence concentration (μg/l [water] or μg/kg [soil or sediment])
C_{Mi}	=	Concentration of *i*th congener in abiotic media (μg/L [water] or μg/kg [soil or sediment])
TEF_i	=	Toxicity equivalency factor (fish) for *i*th congener (unitless)

U.S. EPA OSW assumes that *TEF*s for fish accurately reflect the relative toxicity of PCDD and PCDF congeners to community receptors. This assumption is based on the requirement for congener-specific *TEF*s for this analysis, as an alternative to the overly conservative assumption that all congener concentrations in the media be evaluated directly as 2,3,7,8-TCDD. Evaluation of all congeners directly as 2,3,7,8-TCDD is assumed overly conservative based on the limited evidence of the Ah receptor or TCDD-like toxicity in invertebrates, and that invertebrates appear to be less sensitive to the toxic effects of dioxin-like compounds (WHO 1997). For the same reasons, *TEF* values specific to invertebrate have not been developed; requiring use of the surrogate *TEF* values for fish. The reported findings in WHO (1997) support the use of *TEF*s, in combination with chemical residue data, for the calculation of *TEQ* concentrations in various media, including animal tissues, soil, sediment, and water. However, in relation to the use of *TEF*s for abiotic media, it should be noted that the biological meaning of these values is obscure due to the fact that the assumed biological or toxicological effect is influenced by many physico-chemical factors before uptake occurs (WHO 1997). Nevertheless, *TEF* values can be used as relative measurements of concentrations within media.

Use of the *TEF*s allows for the combined risk resulting from exposure to a mixture of the 17 dioxin-like congeners to be computed assuming that the risks are additive. As discussed in Chapters 5 and 6, risk to the water, sediment, or soil community being evaluated is then subsequently estimated by comparing the media-specific 2,3,7,8-TCDD *TEQ* to the corresponding media-specific toxicity benchmark for 2,3,7,8-TCDD.

2.3.1.3 Exposure Assessment for Class-Specific Guild Measurement Receptors

To evaluate the exposure of class-specific guilds to PCDDs and PCDFs, congener-specific daily doses of all food items (i.e., media, plants, and animals) ingested by a measurement receptor should be converted to a 2,3,7,8-TCDD TEQ daily dose (DD_{TEQ}); which allows for direct comparison to 2,3,7,8-TCDD toxicity benchmarks. The congener-specific daily doses of food items ingested by a measurement receptor should be calculated consistent with the guidance presented in Chapters 4 and 5, and Appendix F, for assessing exposure of class-specific guild measurement receptors to other COPCs. This includes the use of congener-specific media concentrations, congener-specific bioconcentration factors (*BCF*), and congener-specific food chain multipliers (*FCM*). The daily dose of each PCDD and PCDF congener ingested by a measurement receptor should then be multiplied by the congener-specific *TEF*s (see Table 2-3) that correspond to the respective measurement receptor, and summed, to obtain the DD_{TEQ}. Use of the *TEF*s allows for the combined risk resulting from exposure to a mixture of the 17 dioxin-like congeners to be computed assuming that the risks are additive. Following the general guidance provided in Chapters 5 and 6, risk to the class-specific guild being evaluated is then subsequently estimated by comparing the dose ingested term (represented by DD_{TEQ}) of the measurement receptor to the receptor specific toxicity benchmark for 2,3,7,8-TCDD.

The DD_{TEQ} for each measurement receptor should be determined as indicated in the following equation:

$$DD_{TEQ} = \sum DD_i \cdot TEF_{(MeasurementReceptor)} \qquad \text{Equation 2-4}$$

where

DD_{TEQ} = Daily dose of 2,3,7,8-TCDD *TEQ* (μg/kg BW/d)

DD_i	=	Daily dose of *i*th congener (μg/kg BW/d)
TEF	=	Toxicity equivalency factor (specific to measurement receptor) (unitless)

As noted above, the congener-specific daily doses ingested by the measurement receptor should be determined following guidance in Chapter 5 and using equations in Appendix F. These equations include the use of congener-specific *BCF* and *FCM* values. As discussed in Section 2.3.1.4, the limited availability of congener-specific *BCFs* requires that media to receptor *BCF* values for 2,3,7,8-TCDD be utilized in conjunction with congener-specific *BEF* values to obtain estimated congener-specific *BCF* values. The estimation of congener-specific *BCFs* and their resulting numeric values are further discussed in Appendicies C and D. Calculation of a congener-specific daily dose also requires the use of congener-specific *FCMs*. Guidance on the appropriate use of *FCMs* in modeling exposure and congener-specific values are provided in Chapter 5 and Appendix A-2, respectively.

2.3.1.4 Bioaccumulation Equivalency Factors

As discussed in Section 2.3.1.3, modeling the exposure of PCDD and PCDF congeners through the food web requires the quantification of bioaccumulation potential. However, similar to the limited availability of congener-specific toxicity information, measured bioaccumulation data specific to each congener is also limited. Therefore, for use with *TEF*s in the development of wildlife water quality criteria for the Great Lakes, U.S. EPA (1995j) developed bioaccumulation equivalency factors (*BEF*s) as a measure of a congeners bioaccumulation potential relative to 2,3,7,8-TCDD. As indicated in Equation 2-5, *BEF*s are estimated as a ratio between each PCDD and PCDF congener-specific *BASF* to that of 2,3,7,8-TCDD (Lodge et al. 1994; U.S. EPA 1995j).

$$BEF_i = \frac{BSAF_i}{BSAF_{TCDD}} \qquad \text{Equation 2-5}$$

where

BEF_i	=	Bioaccumulation equivalency factor for *i*th congener (unitless)
$BSAF_i$	=	Biota-sediment accumulation factor for *i*th congener (unitless)
$BSAF_{TCDD}$	=	Biota-sediment accumulation factor for 2,3,7,8-TCDD

BEF values reported by U.S. EPA (1995k) for the 17 PCDD and PCDF congeners are provided in Table 2-4. Although developed based on concentration data of PCDDs and PCDFs in sediment and surface water for application of *TEF*s in fish, U.S. EPA OSW assumes that these *BEF*s are applicable to other pathways and receptors. The estimation of PCDD and PCDF congener-specific *BCF* values using *BEF*s is indicated in Equation 2-5. Further discussion and resulting numeric values for congener-specific *BCF*s are provided in Appendicies C and D.

$$BCF_i = BCF_{TCDD} \cdot BEF_i \qquad \text{Equation 2-6}$$

where

BCF_i	=	Media-to-animal or media-to-plant bioconcentration factor for *i*th congener (L/kg [water], unitless [soil and sediment])
BCF_{TCDD}	=	Media-to-receptor BCF for 2,3,7,8-TCDD (L/kg [aquatic receptor], unitless [soil and sediment receptor])
BEF_i	=	Bioaccumulation equivalency factor for *i*th congener (unitless)

TABLE 2-4

PCDD AND PCDF BIOACCUMULATION EQUIVALENCY FACTORS (*BEF*s)

PCDD Congener	Bioaccumulation Equivalency Factor (unitless)	PCDF Congener	Bioaccumulation Equivalency Factor (unitless)
2,3,7,8-TCDD	1.0	2,3,7,8-TCDF	0.80
1,2,3,7,8-PeCDD	0.92	1,2,3,7,8-PeCDF	0.22
1,2,3,4,7,8-HxCDD	0.31	2,3,4,7,8-PeCDF	1.6
1,2,3,6,7,8-HxCDD	0.12	1,2,3,4,7,8-HxCDF	0.076
1,2,3,7,8,9-HxCDD	0.14	1,2,3,6,7,8-HxCDF	0.19
1,2,3,4,6,7,8-HpCDD	0.051	2,3,4,6,7,8-HxCDF	0.67
OCDD	0.012	1,2,3,7,8,9-HxCDF	0.63
		1,2,3,4,6,7,8-HpCDF	0.011
		1,2,3,4,7,8,9-HpCDF	0.39
		OCDF	0.016

Source: U.S. EPA 1995k

2.3.1.5 Fluorine, Bromine, and Sulfur PCDD/PCDF Analogs

U.S. EPA (U.S. EPA 1996l; 1996m) is currently evaluating the potential for the formation of (1) fluorine- and bromine-substituted dioxins and furans, and (2) sulfur analogs of PCDDs and PCDFs. Available information indicates that fluorinated dioxins and furans are not likely to be formed as PICs; however, the presence of free fluorine in the combustion gases may increase the formation of chlorinated dioxins (U.S. EPA 1996l). U.S. EPA OSW is not aware of any studies conducted to evaluate this relationship. Available information indicates the potential for the formation of brominated or chlorobrominated dioxins (U.S. EPA 1996d).

Although chlorinated dibenzothiophenes (the sulfur analogs of dibenzofurans) have been reported to form, no information is available to indicate the formation of chlorinated dioxin thioethers (the sulfur analogs of dibenzo[p]dioxins) (U.S. EPA 1996l). This may be because the carbon-oxygen bond is stronger than the carbon-sulfur bond, and the compound furan (which is part of the dibenzofuran structure) is more stable than thiophene (which is part of the dibenzothiophene structure) (U.S. EPA 1996n). Another possible

reason that chlorinated dioxin thioethers have not been observed is the potential instability of these compounds, which contain two carbon-sulfur bonds in the central ring of the structure (U.S. EPA 1996l). The likelihood of the formation or associated toxicity of these compounds is not currently well understood. Therefore, a quantitative toxicity assessment of fluorine, bromine, and sulfur analogs is not required for inclusion in the risk assessment report. Instead, the uncertainty section of the risk assessment report should discuss the potential for the formation of these analogs. It should be noted that there is currently no U.S. EPA approved method for the sampling or analysis of these dioxin analogs. The use of the method for total organics (see Section 2.2.1.3) is currently recommended to account for the potential presence of these compounds.

TEF values for brominated dioxins or furans have not been developed (U.S. EPA 1994e; WHO 1997). However, the toxicity of bromo- and chlorobromo-substituted dioxin analogs is comparable to that of chlorinated dioxins in short-term toxicity assays (U.S. EPA 1996m).

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Description of any combustion unit-specific operating conditions that may contribute to the formation of dioxins
- Any facility specific sampling information regarding PCDD and PCDF concentrations in air, soil, sediment, water, or biota
- Information regarding the concentration of sulfur, fluorine, and bromine in the combustion unit feed materials

2.3.2 Polynuclear Aromatic Hydrocarbons

Based on their combustion properties and toxicity, U.S. EPA OSW recommends that PAHs be included in every risk assessment. The following are commonly detected PAHs: benzo(a)pyrene (BaP); benzo(a)anthracene; benzo(b)fluoranthene; benzo(k)fluoranthene; chrysene; dibenz(a,h)anthracene; and indeno(1,2,3-cd)pyrene. The general combustion properties and guidance for addressing toxicity of PAHs are discussed in the following paragraph and subsection, respectively.

PAHs are readily formed in combustion units by either (1) dechlorination of other PAHs present in the waste feed or emissions stream (such as dioxins), or (2) the reaction of simple aromatic compounds (benzene or toluene) present in the waste feed or emissions stream. PAHs are well-known as the principal organic components of emissions from all combustion sources, including coal fires (soot), wood fires, tobacco smoke ("tar"), diesel exhaust, and refuse burning (Sandmeyer 1981). They are generally the only chemicals of concern in particulate matter (Manahan 1991), although the presence of metals and other inorganics in the waste feed can add other contaminants of concern. Therefore, based on the toxicity and combustion chemistry of PAHs, the absence of these compounds from stack emissions should always be confirmed via stack gas testing.

2.3.2.1 Exposure Assessment for PAHs

U.S EPA OSW recommends that individual PAH compounds be modeled from the emission source to media (i.e., soil, surface water, soil) and plants, using compound-specific emission rates and fate and transport properties, as required in the media concentration equations (see Chapter 3 and Appendix B). Evaluation of exposure of community and class-specific guild measurement receptors to individual PAHs, should be conducted consistent with guidance provided in Chapters 4 and 5, and utilizing equations in Appendix F.

2.3.3 Polychlorinated Biphenyls

The use and distribution of polychlorinated biphenyls (PCBs) were severely restricted in the United States in the late 1970s—with additional bans and restrictions taking effect over the next decade (ATSDR 1995d). PCBs were produced commercially by the reaction of the aromatic hydrocarbon biphenyl with chlorine gas in the presence of a suitable catalyst, generally ferric chloride or another Lewis acid (ATSDR 1995d). The degree of chlorination was controlled by manipulation of the reaction conditions, including temperature, pressure, and the ratio of the reactants (Erickson 1992; Grayson 1985).

The most commercially useful property of PCBs is that they are chemically stable in relatively adverse conditions, such as a temperature of several hundred degrees in an oxygen-containing atmosphere; the more chlorinated congeners are more resistant to reaction. Therefore, destruction of PCBs by combustion

generally requires conditions of high temperatures (at least 1,200 °C) and an extended contact time (more than 2 seconds) in that temperature with adequate oxygen (Erickson 1992).

Limited data and studies, including laboratory and field, show that PCBs may be formed from the combustion of hazardous waste. Stack tests performed in U.S. EPA Region 10 on a boiler and an incinerator burning waste with 0.07 and 1.4 percent chlorine, respectively, confirmed the presence of PCBs in the stack gases (Kalama Chemical, Inc. 1996; Idaho National Engineering Laboratory 1997). The concentration of detected coplanar PCBs (see definition in Section 2.3.3.1) found in the boiler stack gas was 0.55 ng/dscm @ 7% O_2 at low temperature conditions (1,357° F) and 1.12 ng/dscm @ 7% O_2 at high temperature conditions (1,908° F). The concentration of total PCBs detected in the incinerator stack gas was 211 ng/dscm @ 7% O_2 at low temperature conditions (1,750 °F) and 205 ng/dscm @ 7% O_2 at high temperature conditions (2,075° F). PCBs with more than four chlorines comprised 51 percent of the total PCBs in the low temperature test and 59 percent of the total PCBs in the high temperature test.

Other laboratory studies suggest the possible formation of PCBs as PICs from the combustion of hazardous waste with a high chlorine content. Bergman et al. (1984) heated samples of two chlorinated paraffins (CP) in conditions similar to incinerator conditions. A CP containing 70 percent chlorine did produce PCB (up to 0.3 percent of the amount of CP), as well as chlorinated benzenes (up to 0.5 percent), chlorinated toluenes (up to 0.6 percent), and chlorinated naphthalenes (up to 0.2 percent). Similar treatment of a CP containing 59 percent chlorine produced only chlorinated benzenes (up to 0.1 percent of the amount of CP, based on a detection limit of 0.0005 percent for each individual compound) and almost all of those (about 90 percent) were monochlorobenzene (Bergman et al. 1984). This study indicates that the combustion of highly chlorinated (60 percent or greater chlorine) wastes can produce PCBs.

PCBs should automatically be included as COPCs for combustion units that burn PCB-contaminated wastes or waste oils, highly variable waste streams such as municipal and commercial wastes for which PCB contamination is reasonable, and highly chlorinated waste streams.

Due to the toxicity and uncertainties associated with combustion chemistries the permitting authority may choose to confirm that the absence of these compounds from stack emissions via stack gas testing for units burning hazardous wastes.

2.3.3.1 Exposure Assessment for PCBs

Previous U.S. EPA combustion risk assessment guidance (1994b; 1994d; 1994c; 1994l) has recommended that all PCB congeners (209 different chemicals) be treated in a risk assessment as a mixture having a single toxicity. This recommendation was based on the U.S. EPA drinking water criteria for PCBs (U.S. EPA 1988).

However, since the compilation of U.S. EPA (1988), additional research on PCBs has been reported. The most important result of this research is the demonstration that some of the moderately chlorinated PCB congeners can have dioxin-like effects (U.S. EPA 1992f; U.S. EPA 1994i; ATSDR 1995d; WHO 1997).

WHO (1997) recently convened a conference to discuss the derivation of *TEF*s for humans and wildlife. Conference participants discussed the compilation and review of relevant scientific information on the PCB toxicity to wildlife, and utilized this information to assist in identifying *TEF*s for congeners that can have dioxin-like effects. U.S. EPA OSW believes that these conference proceedings reflect the best available information for screening the ecological risk of PCBs. The following table (see Table 2-5) lists PCB *TEF*s reported for fish, mammals, and birds (WHO 1997).

TABLE 2-5

PCB CONGENER TOXICITY EQUIVALENCY FACTORS (*TEF*s) FOR FISH, MAMMALS, AND BIRDS

PCB Congener	Receptor		
	Fish TEF	Mammals TEF	Birds TEF
3,4,4',5-TCB	0.0005	0.0001	0.1
3,3',4,4'-TCB	0.0001	0.0001	0.05
3,3',4,4',5-PeCB	0.005	0.1	0.1
3,3',4,4',5,5'-HxCB	0.00005	0.01	0.001
2,3,3',4,4'-PeCB	<0.000005	0.0001	0.0001
2,3,4,4',5-PeCB	<0.000005	0.0005	0.0001
2,3',4,4',5-PeCB	<0.000005	0.0001	0.00001
2',3,4,4',5-PeCB	<0.000005	0.0001	0.00001
2,3,3',4,4',5-HxCB	<0.000005	0.0005	0.0001
2,3,3',4,4',5-HxCB	<0.000005	0.0005	0.0001
2,3',4,4',5,5'-HxCB	<0.000005	0.00001	0.00001
2,3,3',4,4',5,5'-HpCB	<0.000005	0.0001	0.00001
2,2',3,3',4,4',5'-HpCB	Not Available	Not Available	Not Available
2,2',3,4,4',5,5'-HpCB	Not Available	Not Available	Not Available

Source: WHO (1997)

The listed congeners have four or more chlorine atoms with few substitutions in the ortho positions (positions designated 2, 2', 6, or 6'). They are sometimes referred to as coplanar PCBs, because the rings can rotate into the same plane if not blocked from rotation by ortho-substituted chlorine atoms. In this configuration, the shape of the PCB molecule is very similar to that of a PCDF molecule. Studies have shown that these dioxin-like congeners can then react with the aryl hydrocarbon receptor; this same reaction is believed to initiate the adverse effects of PCDDs and PCDFs. Additional congeners are suspected of producing similar reactions, but there is not yet enough data to derive *TEF* values for them.

High resolution gas chromatograph test methods (e.g., draft Method 1668), available at most commercial laboratories with dioxin/furan analytical capabilities, should be used to identify the specific concentration of individual coplanar PCBs in stack gas. U.S. EPA OSW recommends that permitting authorities estimate risks to community and class-specific guild measurement receptors from coplanar PCBs by computing a *TEQ* for PCBs, and then comparing to the appropriate toxicity benchmark for 2,3,7,8-TCDD.

The specific guidance, provided in Sections 2.3.1.2 and 2.3.1.2 for evaluating exposure to PCDDs and PCDFs, should be followed in evaluating exposure to dioxin-like PCBs. However, TEF values listed in Table 2-5 should be utilized in the TEQ calculations. Also, since congener-specific fate and transport and bioaccumulation data are not available for each of the PCBs listed in Table 2-5, U.S. EPA OSW recommends that the fate and transport properties for Aroclor 1254 be used in the modeling. This approach is reasonable because approximately 77 percent of Aroclor 1254 is composed of PCB congeners with more than 4 chlorines (Hutzinger et al. 1974).

In addition to the coplanar (dioxin-like) PCB congeners, the remaining PCBs should also be evaluated in the risk assessment consistent with the guidance provided in Chapters 4 and 5. When evaluating PCB mixtures containing isomers with more than 4 chlorines in quantities greater than 0.5 percent of the total PCBs, U.S. EPA OSW recommends that the fate and transport properties for Aroclor 1254 be used in the modeling. As discussed above for evaluating coplanar PCBs, this approach is reasonable because approximately 77 percent of Aroclor 1254 is composed of PCB congeners with more than 4 chlorines (Hutzinger et al. 1974). When assessing risks from PCB mixtures which contain less than 0.5 percent of PCB congeners with more than 4 chlorines, U.S. EPA OSW recommends that the fate and transport properties of Aroclor 1016 be used in the modeling. This approach is reasonable because approximately 99 percent of Aroclor 1016 is comprised of PCB congeners with 4 or less chlorines (Hutzinger et al. 1974).

2.3.4 Nitroaromatics

Careful consideration should be made before the automatic inclusion of nitroaromatic organic compounds, including 1,3-dinitrobenzene; 2,4-dinitrotoluene; 2,6-dinitrotoluene; nitrobenzene; and pentachloronitrobenzene, in risk assessments for combustion units. These compounds or close relatives (such as toluenediamine [TDA] and toluene diisocyanate [TDI]—derivatives of dinitrotoluene) are typically associated with explosives and other highly nitrogenated hazardous wastes. Dinitrotoluene is used to make

two products: trinitrotoluene and TDA. TDA is, in turn, used to make TDI, which readily reacts with water and is, therefore, very unstable at ambient conditions; TDI is typically reacted with a polyol to form polyurethane (PU) plastics.

Combustion properties of these nitroaromatic compounds indicate that they will not be formed as PICs if they are not present in the waste feed stream, mainly because of the thermodynamic and chemical difficulty of adding a nitro group to an aromatic. The process requires that (1) nitronium ions be generated, and (2) an aromatic ring be reacted with the nitronium ion, resulting in the attachment of the nitronium ion to the ring. This reaction process is not likely to occur in a hazardous waste combustion unit because (1) the reaction is typically carried out by using a "nitrating acid" solution consisting of three parts concentrated nitric acid to one part sulfuric acid, and (2) nitronium ions are not usually formed in a combustion unit environment (if they are, a further thermodynamically favorable reaction will occur, thereby eliminating the nitronium ion) (Hoggett et al. 1971; Schofield 1980; March 1985).

Nitroaromatics should be included as COPCs if the hazardous waste feed streams include nitroaromatic compounds or close relatives (TDA and TDI). Also, combustion of feed streams containing unusually high amounts of fuel-bound nitrogen (greater than 5 percent) may lead to increased levels of nitrogenated PICs (U.S. EPA 1994c). Examples of waste feeds identified include heavy distillation fractions and bottoms streams from the production of coal tars and petroleum distillation. Combustion conditions most likely to result in nitrogenated PICs are associated with premature quenching of the primary flame—resulting from low temperature or excess air in the primary combustion chamber of the unit (U.S. EPA 1994c). Sampling for hydrogen cyanide is also recommended (U.S. EPA 1994c).

2.3.5 Phthalates

Careful consideration should be made before the automatic inclusion of phthalates, including bis(2-ethylhexyl)phthalate (BEHP) and di(n)octyl phthalate (DNOP), in risk assessments for combustion units. Among all phthalate plasticizers, BEHP—also referred to as di(2-ethylhexyl)phthalate or dioctyl phthalate)—is produced in the largest volume; it is used in the manufacturing of polyvinyl chloride, which is the most widely produced plastic. DNOP is a plasticizer that is produced in large volumes and is used in the manufacture of plastics and rubber materials. Because plastics have become so widely used in society, phthalate plasticizers such as BEHP and DNOP have become widely distributed in food, water, and the

atmosphere (Howard 1990). Phthalate plasticizers are commonly found in the environment and are practically impossible to avoid, especially at the trace concentrations that modern analyses can detect.

Phthalates are synthesized by reacting alcohol with phthalic anhydride in the presence of an acidic catalyst in a nonaqueous solvent (ATSDR 1993; ATSDR 1995b). Phthalates and their predecessors are readily combusted compounds, as indicated by their flash points of 150 to 225 ^{o}C (NIOSH 1994). There is no apparent mechanism for phthalate PICs to be formed by the combustion of other chemical compounds. Therefore, phthalates are very unlikely to be emissions from a combustion unit, although some degradation products, such as PAHs, are likely to be emitted when phthalates are included in the waste feed. However, facilities that burn plastics or materials with phthalate plasticizers should carefully consider the potential for phthalate plasticizers to exist in the stack gas emissions due to incomplete combustion.

The evaluation of phthalate plasticizers in risk assessments should not be automatically discounted due to the toxicity and biaccumulative potential of these compounds. Moreover, the uncertainties associated with combustion chemistry suggest that the absence of these compounds from stack emissions should always be confirmed via stack gas testing rather than process knowledge or waste feed characterization data. U.S. EPA OSW recommends that careful consideration should be given to including phthalates as COPCs based on the information presented above.

2.3.6 Hexachlorobenzene and Pentachlorophenol

Careful consideration should be made before the automatic inclusion of hexachlorobenzene and pentachlorophenol in risk assessments for combustion units. Hexachlorobenzene and pentachlorophenol, like all chlorinated aromatics, are synthesized by the reaction of elemental chlorine with the parent aromatic (Deichmann and Keplinger 1981; Grayson 1985). The addition of the first chlorine atom to the benzene or phenol molecule is rapid, but further chlorination becomes progressively more difficult, requiring ferric chloride or another Lewis acid catalyst to complete the reaction (March 1985); therefore, these chlorinated compounds are difficult to make under controlled conditions. Hexachlorobenzene, but not pentachlorophenol, has been reported in emissions from the combustion of municipal solid waste and from other processes (such as the chlorination of wood pulp) that also produce PCDDs and PCDFs (ATSDR 1994a; ATSDR 1994b). Hexachlorobenzene is an impurity in pentachlorophenol while pentachlorophenol is formed from hexachlorobenzene in some factories (ATSDR 1994a; ATSDR 1994b). The combustion

properties of these chlorinated compounds indicate that they are not likely to be formed as PICs if they are not present in the waste feed stream.

Hexachlorobenzene and pentachlorophenol should be included as COPCs for units that burn waste feeds containing hexachlorobenzene and pentachlorophenol, wood preservatives, pesticides, and highly variable waste streams such as municipal solid waste. However, precluding these compounds from analytical testing during the trial burn based on process knowledge and waste feed characterization is not recommended. Because PCDDs and PCDFs can be formed from fly ash-catalyzed reactions between halogens and undestroyed organic material from the furnace, U.S. EPA guidance (U.S. EPA 1993h; 1994d) has recommended that potential precursor compounds be included in the risk assessment and trial burn (see Section 2.3). These precursor compounds may include chlorinated phenols (such as pentachlorophenol) and chlorinated aromatics (such as hexachlorobenzene). Furthermore, the toxicity and uncertainties associated with combustion chemistry suggest that the absence of these compounds from stack emissions should always be confirmed via stack gas testing. U.S. EPA OSW recommends that careful consideration should be given to including hexachlorobenzene and pentachlorophenol as COPCs based on the information presented above.

2.3.7 Metals

U.S. EPA OSW recommends that the following inorganic substances be considered for evaluation in the risk assessment: aluminum, antimony, arsenic, barium, beryllium, cadmium, hexavalent chromium, copper, lead, mercury (elemental and divalent), nickel, selenium, silver, thallium, and zinc. All of these substances, except aluminum, copper, nickel, selenium, and zinc, are regulated by 40 CFR Part 266, Subpart H (the BIF regulations). In the case of metals not regulated by the BIF regulations, U.S. EPA has recommended that these metals be evaluated, to determine whether additional terms and conditions should be incorporated into the permit, by using U.S. EPA's omnibus authority provided under 40 CFR Part 270.32(b)(2) (U.S. EPA 1992c). Facilities may also apply the BIF regulation Tier I assumptions, that assume all metals in the waste feed pass through the combustion unit and APCS and are passed through to the emission stream (U.S. EPA 1992e).

It should be noted, that the presence of metals in the combustion unit's feed stream is not required for inclusion in the risk assessment. Although metals cannot be formed as PICs, U.S. EPA OSW is aware of combustion units with metal emissions resulting from waste feed leaching of stainless steel feed piping.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Waste feed, raw material, and secondary fuel stream analytical data
- Metal emission rate sampling data or assumptions based on waste feed data
- Explanations for excluding specific metals from evaluation in the risk assessment

The following subsections provide additional information regarding U.S. EPA-recommended procedures for evaluating metals—chromium, mercury, and nickel—that may be specifically altered during the combustion process or require specific considerations in the risk assessment.

2.3.7.1 Chromium

The oxidation state of chromium is a crucial issue in evaluating the toxicity of this metal and the risks associated with exposure. Hexavalent chromium (Cr^{+6}) is the most toxic valence state of chromium. Trivalent chromium (Cr^{+3}), a commonly found less oxidized and toxic form of chromium, is more commonly found in the environment. U.S. EPA (1990c; 1990d) has indicated that chromium emitted from a combustion unit is not likely to be in the hexavalent form; however, there is not sufficient evidence to reliably estimate the partitioning of chromium emissions into these two valence states. Also, media-specific chromium speciation information is often difficult to obtain within the scope of a screening risk assessment. However, U.S. EPA OSW recognizes that chromium may exist partially or in some cases entirely as trivalent chromium in various media. Therefore, unless site-sampling or process-specific information is provided to support a less conservative approach, the worst-case assumption—that 100 percent of the facility chromium emissions are in the hexavalent form—should be used as the initial assumption that all exposure is to hexavalent chromium.

The assumption that receptors are exposed to hexavalent chromium should be maintained in the absence of site specific data. However, permitting authorities may prepare supplemental calculations (that is, in addition to the site-specific data described above) considering chromium speciation at the points of potential exposure.

2.3.7.2 Mercury

Consistent with previous U.S. EPA combustion risk assessment guidance (U.S. EPA 1993h, 1994d, 1994c, 1994l), U.S. EPA OSW recommends that mercury be evaluated as COPCs in the risk assessment. Air emissions of mercury contribute to local, regional, and global deposition. The U.S. Congress explicitly found this to be the case and required U.S. EPA to prioritize maximum achievable control technology (MACT) controls for mercury (U.S. Congress 1989).

Anthropogenic mercury releases are thought to be dominated on the national scale by industrial processes and combustion sources that release mercury into the atmosphere (U.S. EPA 1997b). Stack emissions containing mercury include both vapor and particulate forms. Vapor mercury emissions are thought to include both elemental (Hg^0) and oxidized (e.g., Hg^{+2}) chemical species, while particulate mercury emissions are thought to be composed primarily of oxidized compounds due to the relatively high vapor pressure of elemental mercury (U.S. EPA 1997b). While coal combustion is responsible for more than half of all emissions of mercury in the U.S. anthropogenic sources, the fraction of coal combustion emissions in oxidized form is thought to be less that from waste incineration and combustion (U.S. EPA 1997b).

The analytical methods for mercury speciation of exit vapors and emission plumes are being refined, and there is still controversy in this field. Chemical reactions occurring in the emission plume are also possible. The speciation of mercury emissions is thought to depend on the fuel used, flue gas cleaning, and operating temperatures. The exit stream is thought to range from almost all divalent mercury to nearly all elemental mercury; with true speciation of mercury emissions from the various source types still uncertain and thought to vary, not only among source types, but also for individual plants as feed stock and operating conditions change (U.S. EPA 1997b). Most of the total mercury emitted at the stack outlet is found in the vapor phase; although exit streams containing soot or particulate can bind up some fraction of the mercury (U.S. EPA 1997b). Total mercury exiting the stack is assumed to consist of elemental and divalent species,

with no emissions of methylmercury assumed. The divalent fraction is split between vapor and particle-bound phases (Lindqvist et al. 1991). Much of the divalent mercury is thought to be mercuric chloride ($HgCl_2$) (U.S. EPA 1997b); this is particularly the case for the combustion of wastes containing chlorine.

It should be noted that data on mercury speciation in emissions exiting the stack is very limited, as well as, the behavior of mercury emissions close to the point of release has not been extensively studied. This results in a significant degree of uncertainty implicit in modeling of mercury emissions. Additional examples of uncertainties include the precision of measurement techniques, estimates of pollution control efficiency, limited data specific to source class and activity level. Discussions of uncertainty and sensitivity analyses of several of the assumptions used in the modeling of mercury emissions are presented in the *Mercury Study Report to Congress* (U.S. EPA 1997b).

Phase Allocation and Speciation of Mercury Exiting the Stack

As discussed above, stack emissions are thought to include both vapor and particle-bound forms; and speciated as both divalent and elemental mercury. Based on review of mercury emissions data presented for combustion sources in U.S. EPA (1997b) and published literature (Peterson et al. 1995), estimates for the percentage of vapor and particle-bound mercury emissions range widely from 20 to 80 percent. Therefore, at this time U.S. EPA OSW recommends a conservative approach that assumes phase allocation of mercury emissions from hazardous waste combustion of 80 percent of the total mercury in the vapor phase and 20 percent of total mercury in the particle-bound phase. This allocation is:

- Consistent with mercury emissions speciation data for hazardous waste combustion sources reported in literature (Peterson et al. 1995); and
- Believed to be reasonably conservative, since it results in the highest percentage of total mercury being deposited in proximity to the source, and therefore, indicative of the maximum exposure.

As indicated in the global cycle mass percentages in Figure 2-4, mercury exits the stack in both the elemental and divalent vapor forms. Based on U.S. EPA (1997b), a vast majority of mercury exiting the stack does not readily deposit and is transported outside of the U.S. or vertically diffused to the free atmosphere to become part of the global cycle (see Figure 2-4). The divalent form emitted, either in the

vapor phase or particle-bound, are thought to be subject to much faster atmospheric removal than elemental mercury (Lindberg et al. 1992; Peterson et al. 1995; and Shannon and Voldner 1994). In addition, vapor phase divalent mercury is thought to be more rapidly and effectively removed by both dry and wet deposition than particle-bound divalent mercury, as a result of the reactivity and water solubility of vapor divalent mercury (Lindberg et al. 1992; Peterson et al. 1995; and Shannon and Voldner 1994).

Vapor Phase Mercury

As illustrated in Figure 2-4, of the 80 percent total mercury in the vapor phase, 20 percent of the total mercury is in the elemental vapor form and 60 percent of the total mercury is in the divalent vapor form (Peterson et al. 1995). A vast majority (assumed to be 99 percent) of the 20 percent vapor phase elemental mercury does not readily deposit and is transported outside of the U.S. or is vertically diffused to the free atmosphere to become part of the global cycle (U.S. EPA 1997b). Only a small fraction (assumed to be one percent) of vapor-phase elemental mercury either is adsorbed to particulates in the air and is deposited or converted to the divalent form to be deposited (assumed to be deposited as elemental mercury, see Figure 2-4). Of the 60 percent vapor phase divalent mercury, about 68 percent is deposited and about 32 percent is transported outside of the U.S. or is vertically diffused to the free atmosphere to become part of the global cycle (U.S. EPA 1997b).

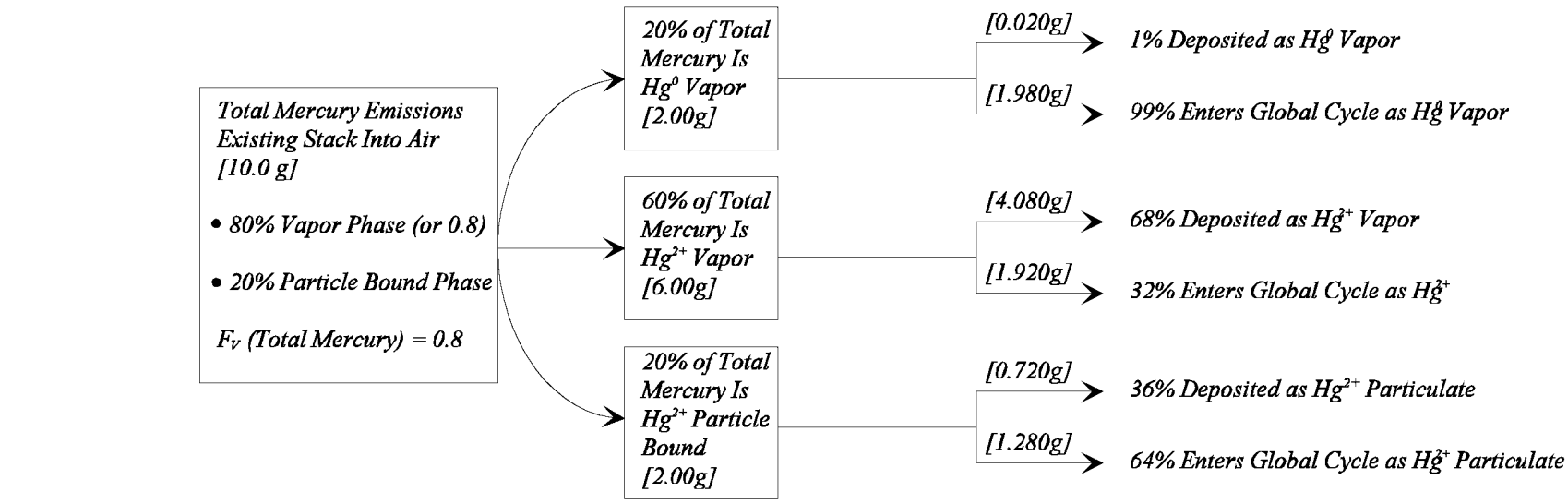
Particle-bound Mercury

Of the 20 percent of the total mercury that is particle-bound, 99 percent (assumed to be 100 percent in Figure 2-4) is in the divalent form. U.S. EPA (1997b) indicates that only 36 percent of the particle-bound divalent mercury is deposited, and the rest is either transported outside of the U.S. or is vertically diffused to the free atmosphere to become part of the global cycle.

Deposition and Modeling of Mercury

Consistent with U.S. EPA (1997b) and as shown in Figure 2-4, it is assumed that deposition to the various environmental media is entirely divalent mercury in either the vapor or particle-bound form. Without consideration of the global cycle, mercury speciations will result in 80 percent of the total mercury emitted being deposited as divalent mercury and the remaining 20 percent being deposited as elemental mercury.

FIGURE 2-4
PHASE ALLOCATION AND SPECIATION
OF MERCURY IN AIR



LEGEND

Hg^0 - Elemental Mercury
Hg^{2+} - Divalent Mercury
[ ] - Example Mass Allocation

Without Consideration of Global Cycle
- *80% of Total Mercury Emitted is Deposited as Hg^{2+} [(6g + 2g) / 10g]*
- *20% of Total Mercury Emitted is Deposited as Hg^0 [2g / 10g]*

Calculated F_V
- *F_V (Hg^{2+}) = [6g / (6g +2g)] = 0.75*
- *F_V (Hg^0) = [2g / 2g] = 1.0*

With Consideration of Global Cycle
- *48% of Total Mercury Emitted is Deposited as Hg^{2+} [(4.08g + 0.72g) / 10g]*
- *0.2% of Total Mercury Emitted is Deposited as Hg^0 [0.02g / 10g]*

Calculated F_V
- *F_V (Hg^{2+}) = [4.08g / (4.08g + 0.72g)] = 0.85*
- *F_V (Hg^0) = [0.02g / (0.02g + 0g)] = 1.0*

Compound Specific Emission Rate Q
- *Actual Q (Hg^{2+}) = 48% * Q (Total Mercury)*
- *Actual Q (Hg^0) = 0.2% * Q (Total Mercury*

U.S. EPA OSW recommends utilizing the percentages provided in U.S. EPA (1997b) to account for the global cycle, the percentage of total mercury deposited is reduced to a total of 48.2 percent (40.8 percent as divalent vapor, 7.2 percent as divalent particle-bound, and 0.2 percent as elemental vapor). As discussed in Appendix A-2, these speciation splits result in fraction in vapor phase (*Fv)* values of 0.85 (40.8/48.2) for divalent mercury, and 1.0 (0.2/0.2) for elemental mercury. Also, to account for the remaining 51.8 percent of the total mercury mass that is not deposited, the deposition and media concentration equations (presented in Appendix B), multiply the compound-specific emission rate (*Q*) for elemental mercury by a default value of 0.002; and divalent mercury by a default value of 0.48.

Consistent with U.S. EPA (1997b) and as shown in Figure 2-4, it is assumed that deposition to the various environmental media is entirely divalent mercury in either the vapor or particle-bound form. Deposited divalent mercury is also considered as a source of methyl mercury, which is assumed as a media-specific percentage of the total mercury deposited.

Also, only a small fraction (assumed to be one percent) of elemental mercury is in the vapor phase and is assumed to be deposited in its original form. Therefore, any resulting exposure to elemental mercury is considered to be much less significant, and will not be considered in the pathways of the ecological risk assessment.

Appendix A-2 provides the parameter values specific to the various forms of mercury, and Appendix B provides media concentration equations for modeling mercury through the exposure pathways assuming steady-state conditions.

Methylation of Mercury

The net mercury methylation rate (the net result of methylation and demethylation) for most soils appears to be quite low; with much of the measured methyl mercury in soils potentially resulting from wet deposition (U.S. EPA 1997b). Consistent with U.S. EPA (1997b), a fraction of the divalent mercury that is deposited is assumed to speciate to organic mercury (methyl mercury) in soil. In soil, 98 percent of total mercury is assumed to be divalent mercury and the remaining mass as methyl mercury (U.S. EPA 1997b). A significant and important exception to mercury methylation rate being low in soils appears to be wetland soils. Wetlands appear to convert a small but significant fraction of the deposited mercury into methyl mercury; which can be

exported to nearby water bodies and potentially bioaccumulated in the aquatic food chain (U.S. EPA 1997b). Therefore, the assumed percentage of methyl mercury in wetland soils may be higher than the 2 percent assumed for non-wetland soils, and may closer approximate the 15 percent assumed for sediments.

Both watershed erosion and direct atmospheric deposition can be important sources of mercury to a water body (U.S. EPA 1997b). There appears to be a great deal of variability in the processing of mercury among water bodies. This variability is primarily a result of the characteristically wide range of chemical and physical properties of water bodies that influence the levels of methylated mercury. Some of the mercury entering the water body is methylated predominately through biotic processes (U.S. EPA 1997b). In the absence of modeling site-specific water body properties and biotic conditions, consistent with U.S. EPA (1997b), U.S. EPA OSW recommends 85 percent of total mercury in surface water is assumed to be divalent mercury and the remaining mass as methyl mercury.

For most environmental systems, the literature suggests that various physical and chemical conditions may influence the methylation of mercury. Consideration of these conditions, and the magnitude of their potential impact, may be required in some cases to assess the potential for over or under predicting mercury methylation in media and subsequent biotransfer up the food chain. Due to the extreme variance between environmental systems modeled, and at times disagreement, identified in literature reviewed regarding the quantitative influence of specific conditions on methylation, U.S. EPA OSW recommends that extensive research of literature, specific to the conditions prevalent at the site, be conducted before application and deviation from the conservative assumptions recommended above. The following table summarizes the qualitative effect some of the physical and chemical conditions, as reported in literature, may have on methylating:

Physical or Chemical Condition	Qualitative Influence on Methylation	Referenced Literature
Low dissolved oxygen	Enhanced methylation	Rudd et al. 1983; Parks et al. 1989
Decreased pH	Enhanced methylation in water column	Xun 1987; Gilmour and Henry 1991; Miskimmin et al. 1992
Decreased pH	Decreased methylation in sediment	Ramlal et al. 1985; Steffan et al. 1988
Increased dissolved organic carbon (DOC)	Enhanced methylation in sediment	Chois and Bartha 1994
Increased dissolved organic carbon (DOC)	Decreased methylation in water column	Miskimmin et al. 1992
Increased salinity	Decreased methylation	Blum and Bartha 1980
Increased nutrient concentrations	Enhanced methylation	Wright and Hamilton 1982; Jackson 1986; Regnell 1994; Beckvar et al. 1996
Increased selenium concentrations	Decreased methylation	Beckvar et al. 1996
Increased temperature	Enhanced methylation	Wright and Hamilton 1982; Parks et al. 1989
Increased sulfate concentrations	Enhanced methylation	Gilmour and Henry 1991; Gilmour et al. 1992
Increased sulfide concentrations	Enhanced methylation	Beckvar et al. 1996

To account for methylation of mercury in the media and its subsequent biotransfer assuming steady-state conditions, the deposition and media concentration equations (presented in Appendix B) have been modified specifically for modeling methyl mercury. Appendix A-2 provides the parameter values specific for methylmercury, and additional discussion and reference on their origin.

As noted above, methylation can be highly variable between environmental systems. This results in a significant degree of uncertainty implicit in modeling of mercury methylation. To expand on the qualitative information presented in the above table, and better understand conditions that may influence mercury methylation specific to a site, U.S. EPA OSW recommends review of information on this subject presented in the *Mercury Study Report to Congress* (U.S. EPA 1997b).

Exposure Assessment for Mercury

For assessing exposure of community and class-specific guild measurement receptors to mercury, guidance provided in Chapters 4 and 5 should generally be followed. However, special consideration is required in evaluating the various forms of mercury modeled to the point of exposure.

To evaluate exposure of water, sediment, and soil communities to mercury, species-specific concentrations of divalent mercury and methyl mercury, in the respective media to which the community is exposed, should be directly compared to toxicity benchmarks specific to those compounds. The species-specific media concentrations should be calculated using equations and guidance presented in Chapter 3 and Appendix B. Media-specific toxicity benchmarks for divalent and methyl mercury are provided in Appendix E.

To evaluate the exposure of class-specific guilds to mercury, the media-specific concentrations of both divalent and methyl mercury should be modeled as independent COPCs through the food web, assuming no methylation of divalent mercury to the methyl mercury form within organisms. Therefore, the daily doses of all food items (i.e., media, plants, and animals) ingested by a measurement receptor should be considered for both divalent and methyl mercury, and compared to the respective toxicity benchmarks that are representative of the measurement receptor (see Appendix E). The daily doses of food items ingested by a measurement receptor should be calculated consistent with the guidance presented in Chapters 4 and 5, and Appendix F, for assessing exposure of class-specific guild measurement receptors to other COPCs. This includes the use of species-specific media concentrations, and methyl mercury bioconcentration factors (*BCF*) and food chain multipliers (*FCM*).

Conclusion

In the event risks associated with mercury exceed target levels based on modeling with equations and initial conservative assumptions presented in this guidance, the permitting authority may approve use of more complex models that utilize more extensive site-specific data to predict transformation of chemical forms and biotransfer of mercury for evaluation at points of potential exposure. For example, the draft version of the ISCST3 dry gas algorithm for estimating dry gas deposition may be utilized. This draft model can be found

on the SCRAM bulletin (see Chapter 3); and specific default parameter values for mercury are presented in U.S. EPA (1997b). While this guidance does not address what models should be used or how data to support such models should be collected, the decision to use site-specific mercury models in a risk assessment is not precluded just because it is different; nor does this guidance automatically approve the use of such models. A permitting authority that chooses to use complex mercury models should carefully identify and evaluate their associated limitations, and clearly document these limitations in the uncertainty section of the risk assessment report.

U.S. EPA OSW encourages all facilities to implement a combination of waste minimization and control technology options to reduce mercury emission rates on an ongoing basis. Realistic expectations for mercury emission reduction efforts may be established by considering various technology-based mercury emission limits that apply to waste combustors (for example, standards for European combustors, the proposed MACT standards for hazardous waste combustors, or the MACT standards for municipal waste combustors). U.S. EPA OSW acknowledges that site-specific risk assessments as currently conducted may not identify the entire potential risk from mercury emissions. Mercury that does not deposit locally will ultimately enter the global mercury cycle for potential deposition elsewhere.

2.3.8 Particulate Matter

PM is all condensed material suspended in air that has a mean aerodynamic diameter of 10 micrometers or less (PM10). PM can be classified as aerosols, dusts, fogs, fumes, mists, smogs, or smokes, depending on its physical state and origin. Anecdotal evidence suggests that uncontrolled particulate emissions from coal-burning industries has adversely affected local populations of wildlife (U.S. Fish and Wildlife Service [U.S. FWS] 1980). For wildlife, PM can adsorb to external surfaces or membranes, for example causing corneal damage. Wildlife exposure can also occur through ingested of contaminated food, water, and hair (through grooming) (U.S. FWS 1980). However, PM dose-response information to evaluate risk of particulate matter to ecological receptors is limited. For this reason, U.S. EPA OSW does not recommend that PM be evaluated as a separate COPC in a risk assessment. However, PM is useful as an indicator parameter for other contaminants because it can be measured in real time and is sensitive to changes in combustion conditions.

2.3.9 Hydrogen Chloride/Chlorine Gas

Hydrogen chloride (which becomes hydrochloric acid when dissolved in water) and chlorine are two of the major products of the chemical industry, with uses too numerous to list. When chlorine gas dissolves in water (whether during drinking water treatment or when someone inhales chlorine), it hydrolyzes to form equal amounts of hydrochloric acid and hypochlorous acid.

Hydrogen chloride, as all other strong acids and bases, is an irritant on contact; adverse effects are seen only in the upper respiratory tract (including the nose, mouth, and throat). High concentrations can become corrosive and destroy tissues, producing chemical burns. Unless it is highly concentrated, ingested hydrochloric acid has only minimal adverse effects.

Because of the high concentrations of these compounds needed to produce observable effects, they are not expected to pose an ecological risk. Therefore, U.S. EPA OSW does not recommend that hydrogen chloride and chlorine gas be included as separate COPCs in the risk assessment.

2.3.10 Endocrine Disruptors

Endocrine disruptors are chemical compounds that interfere with the endocrine system's normal function and homeostasis in cells, tissues, and organisms. It has been hypothesized by U.S. EPA OSW that endocrine disruptors adversely affect the reproductive system by interfering with production, release, transport, receptor binding action, or elimination of natural blood-borne hormones and ligands.

Several studies have been conducted and serve as the basis for further experimentation to determine whether the hypothesis is correct. These studies include (1) wildlife reproduction (feminization of birds, alligators, and certain terrestrial mammals), (2) wildlife population ecology (population decline), (3) human reproductive physiology (decreased sperm count in males in industrialized nations), (4) molecular biology (data on receptor-mediated mode of action), and (5) endocrinology (increased understanding of mechanisms of hormone regulation and impacts of perturbations).

Some have attempted to classify chemical compounds as endocrine disruptors; however, several problems have been encountered. Only limited empirical data are available to support the designation of specific

chemicals as endocrine disruptors, and some of the data are conflicting. An absence of a clear structure-activity relationship is evident among the diverse groups of chemicals considered as endocrine disruptors. There is a lack of unifying dose-response relationship among the diverse group of chemicals. Also, multiple modes of action for chemicals are currently considered as endocrine disruptors.

Because the information currently available on endocrine disruptors is inconsistent and limited, U.S. EPA has not yet developed a methodology for quantitative assessments of risk resulting from potential endocrine disruptors (U.S. EPA 1996d). Currently, no quantitative U.S. EPA methods exist to specifically address the effects of endocrine disrupters in a risk assessment. Because the methods for addressing endocrine disrupters are developing at a rapid pace, permits writers and risk assessors should contact the Economics, Methods and Risk Analysis Division (EMRAD) of the Office of Solid Waste for the latest policy on how to deal with endocrine disrupters in site specific risk assessments. Additional information can also be obtained from review of available publications (e.g., EPA Special Report on Endocrine Disruption) at the web site "www.epa.gov/ORD/WebPubs/endocrine/".

2.3.11 Radionuclides

Radionuclides exist in (1) naturally occurring radioactive materials such as coal and other rocks, as (2) radioactive by-products of industrial processes. This risk assessment guidance does not consider the naturally occurring radioactive materials such as uranium and thorium (and their decay elements) based on U.S. EPA doctrine and technical limitations for measuring such low levels. However, radioactive wastes and materials, as defined by the U.S. Nuclear Regulatory Commission (NRC) and the U.S. Department of Energy (DOE), are subject to evaluation through interagency agreements on this subject. The U.S. NRC considers "radioactive waste" as waste that is, or contains, by-product material, source material, or special nuclear material (as defined in 10 CFR Part 20.1003). The U.S. NRC considers "mixed waste" as waste that is radioactive waste and hazardous waste defined by U.S. EPA. Radioactive and mixed waste must be handled in accordance with all relevant regulations, including U.S. EPA and U.S. NRC (10 CFR Part 20.2007) regulations. In particular, U.S. NRC licensees must comply with 10 CFR Part 20.2004—"Treatment or Disposal by Incineration"—and applicable U.S. EPA regulations.

U.S. EPA OSW recommends that the combustion of mixed waste and radioactive material should be evaluated in the risk assessment. Direct radiation (e.g., radiation from sealed sources such as instruments

that are not released to the environment) does not need to be evaluated in the risk assessment. Risk from both radiological and non-radiological contaminants should be presented along side each other in a risk summary table. Results should include a discussion of additivity and the uncertainties of additivity when combining risks from radiological and non-radiological contaminants. A radionuclide should be included as a COPC if it is in the combustion unit's waste feed.

U.S. EPA OSW recommends using the ISCST3 air dispersion model, utilizing the exponential decay option to calculate air concentrations and ground deposition rates. Intake should then be calculated with appropriate exposure scenario equations and parameters. ISCST3 is a good choice for facilities with multiple sources, complex terrain, building downwash and wet/dry deposition requirements.

A special consideration in integrating radioactive materials into risk calculations is related to decay and ingrowth of radionuclides, especially the few decay processes that involve a change of state. Decay should always be considered, both over the air transport time and the surface exposure duration. Ingrowth may be important, and special care must be taken in the use of radionuclide slope factors that include contributions from daughters ('+D" slope factors). Ingrowth involving change of physical states is another situation that will require special handling in the fate and transport modeling. For instance, solid radium-226 decays to gaseous radon-222, which then decays through solid polonium-218 to further decay elements.

Equations for fate and transport of radionuclides in soil and water should be consistent with those presented for non-radionuclides factoring in decay (and ingrowth if applicable). Food chain biotransfer parameters necessary to determine food concentrations are available in the *Handbook of Parameter Values for the Prediction of Radionuclide Transfer in Temperate Environments; IAEA Technical Report Series No. 364* (International Atomic Energy 1994).

Because the information currently available on ecological fate and effects for radionuclides is very limited, U.S. EPA OSW has not yet developed a methodology for quantitative assessments of ecological risk resulting from exposure. Ecological screening levels currently being used in some regions include 1 rad/day for aquatic receptors, based on population effects, (National Council on Radiation Protection and Measurements 1991), and 0.1 rad/day for terrestrial receptors (with the exception of pine trees and mammalian embryos) (International Atomic Energy Agency 1992). Additional references on evaluating ecological exposures to radiation include Barnthouse (1995) and Blaylock et al. (1993).

USER NOTE

Prescriptive methodology for calculating risk from combustion facilities burning mixed waste is beyond the scope of the current document. The above information is provided to outline the methodology recommended by U.S. EPA OSW.

2.4 ESTIMATES OF COPC CONCENTRATIONS FOR NON-DETECTS

The lowest level of an analyte that can be detected using an analytical method is generally termed the "detection limit." One particularly difficult issue is the treatment of data in the risk assessment that are reported as below the "detection limit." The following subsections (1) define commonly reported "detection limits," (2) describe use in the risk assessment of data reported as non-detect, (3) describe statistical distribution techniques applied to address this issue, (4) summarize U.S. EPA OSW recommendations regarding quantification of non-detect issues in preparation of a risk assessment, and (5) clarify data flagged as estimated maximum possible concentration (EMPC) in the risk assessment.

2.4.1 Definitions of Commonly Reported Detection Limits

U.S. EPA's commonly-used definition for the detection limit for non-isotope dilution methods has been the method detection limit (MDL), as promulgated in 40 CFR Part 136, Appendix B (U.S. EPA 1995i). A level above the MDL is the level at which reliable quantitative measurements can be made; generically termed the "quantitation limit" or "quantitation level." In practice, numerous terms have been created to describe detection and quantitation levels. The significance and applicability of the more widely reported of these detection and quantitation levels by analytical laboratories are summarized below. These levels—listed generally from the lowest limit to the highest limit—include the following:

- Instrument Detection Limit (IDL) is the smallest signal above background that an instrument can reliably detect, but not quantify. Also, commonly described as a function of the signal-to-noise (S/N) ratio.

- Method Detection Limit (MDL) is the minimum concentration of a substance that can be measured (via non-isotope dilution methods) and reported with 99 percent confidence that the analyte concentration is greater than zero, and is determined from analysis of a sample in a specific matrix type containing the analyte. The MDL is considered the lowest level at which a compound can be reliably detected. The MDL is based on statistical analyses of laboratory data. In practice, the MDLs are determined on analytical reagents (e.g., water)

and not on the matrix of concern. MDLs for a given method, are laboratory and compound specific.

> To determine the MDL as specified in 40 CFR Part 136, Appendix A, for example, at least seven replicate samples with a concentration of the compound of interest near the estimated MDL are analyzed. The standard deviation among these analyses is calculated and multiplied by 3.14. The result of the calculation becomes the MDL. The factor of 3.14 is based on a t-test with six degrees of freedom and provides a 99 percent confidence that the analyte can be detected at this concentration (U.S. EPA 1995i).
>
> It should be noted that 40 CFR Part 136 is specific to the Clean Water Act, and therefore, it identifies the use of water as the matrix for the MDL determination. The MDL was promulgated in 1984, and is incorporated in more than 130 U.S. EPA analytical methods for the determination of several hundred analytes.

- Reliable Detection Level (RDL) is a detection level recommended by the National Environmental Research Laboratory in Cincinnati. It is defined as 2.623 times the MDL (U.S. EPA 1995i). The RDL is a total of 8 standard deviations above the MDL developmental test data (3.14 times 2.623).

- Estimated Detection Limit (EDL) is a quantitation level defined in SW-846 that has been applied to isotope dilution test methods (e.g., SW-846 Method 8290). A variation of the SW-846 defined EDL is also commonly reported by commercial laboratories, however, with the addition of a multiplication factor that generally elevates the EDL value by 3.5 to 5 times that of the SW-846 definition. Commercial laboratories sometimes report EDLs for non-isotope dilution methods such as SW-846 Method 8270, even though an EDL is not defined by the method.

  As defined in SW-846: The EDL is defined in SW-846 (presented in various methods, e.g., Method 8280A) as the estimate made by the laboratory of the concentration of a given analyte required to produce a signal with a peak height of at least 2.5 times the background signal level. The estimate is specific to a particular analysis of the sample and will be affected by sample size, dilution, etc. The presented equation defining EDL is as follows:

$$EDL = \frac{2.5 \cdot Q_{is} \cdot (H_n^1 + H_n^2) \cdot D}{V \cdot (H_{is}^1 + H_{is}^2) \cdot RF_n} \qquad \text{Equation 2-7}$$

where

EDL	=	Estimated detection limit (ng/L)
2.5	=	Peak height multiplier (unitless)
Q_{is}	=	Nanograms of the appropriate internal standard added to the sample prior to extraction (ng)

H_n^1 *and* H_n^2	=	The peak heights of the noise for both of the quantitation ions of the isomer of interest
H_{is}^1 *and* H_{is}^2	=	The peak heights of both the quantitation ions of the appropriate internal standards
D	=	Dilution factor - the total volume of the sample aliquot in clean solvent divided by the volume of the sample aliquot that was diluted (unitless)
V	=	Volume of sample extracted (L)
RF_n	=	Calculated relative response factor from calibration verification (unitless)

Common commercial laboratory practice: The EDL, generally reported by commercial laboratories, is defined as the detection limit reported for a target analyte that is not detected or presents an analyte response that is less than 2.5 times the background level. The area of the compound is evaluated against the noise level measured in a region of the chromatogram clear of genuine GC signals times an empirically derived factor. This empirical factor approximates the area to height ratio for a GC signal. This factor is variable between laboratories and analyses performed, and commonly ranges from 3.5 to 5. The equation is as follows:

$$EDL = \frac{2.5 \cdot Q_{\beta} \cdot (F \cdot H) \cdot D}{W \cdot A_{\beta} \cdot RRF_{\sigma}} \qquad \text{Equation 2-8}$$

where

EDL	=	Estimated detection limit
2.5	=	Minimum response required for a GC signal
Q_{β}	=	The amount of internal standard added to the sample before extraction
F	=	An empirical factor that approximates the area to height ratio for a GC signal
H	=	The height of the noise
D	=	Dilution factor
W	=	The sample weight or volume
RRF_{σ}	=	The mean analyte relative response factor from the initial calibration

- Practical Quantitation Limit (PQL) is a quantitation level that is defined in 50 FR 46908 and 52 FR 25699 as the lowest level that can be reliably achieved with specified limits of precision and accuracy during routine laboratory operating conditions (U.S. EPA 1992g; 1995i). The PQL is constructed by multiplying the MDL, as derived above, by a factor (subjective and variable between laboratories and analyses performed) usually in the range of 5 to 10. However, PQLs with multipliers as high as 50 have been reported (U.S. EPA 1995i).

The PQL has been criticized because of the ambiguous nature of the multiplier and because the resulting levels have been perceived as too high for regulatory compliance purposes (U.S. EPA 1995i).

- Target Detection Limit (TDL) is a quantitation level constructed similar to the PQL.
- Reporting Limit (RL) is a quantitiation level constructed similar to the PQL.
- Estimated Quantitation Limit (EQL) is a quantitiation level constructed similar to the PQL.
- Sample Quantitation Limit (SQL) is a quantitation level that is sample-specific and highly matrix-dependent because it accounts for sample volume or weight, aliquot size, moisture content, and dilution. SQLs for the same compound generally vary between samples as moisture content, analyte concentration, and concentrations of interfering compounds vary. The SQL is generally 5 to 10 times the MDL, however, it is often reported at much higher levels due to matrix interferences.
- Contract Required Quantitation Limit (CRQL)/Contract Required Detection Limit (CRDL) is a quantitation pre-set by contract, which may incorporate U.S. EPA (1986b) SW-846 methods, Office of Water methods, or other methods deemed necessary to meet study objectives. These limits are typically administrative limits and may actually be one or two orders of magnitude above the MDL.

2.4.2 Use In the Risk Assessment of Data Reported As Non-Detect

In collecting data for use in risk assessments or in setting regulatory compliance levels, the permitting authority is often faced with data quality objectives that require analyses near or below analytical detection or quantitation levels. In such situations, permittees often argue that the detection levels should be set with a large factor of certainty in order to be confident that measurements are reliable. Environmental groups frequently argue that a level of zero or a level at which a single researcher can demonstrate that the compound can be detected should be used as the set level. Because measurements made below analytical detection and quantitation levels are associated with increased measurement uncertainty, an understanding of these levels is important to the comprehension of the impact they may have when they are applied.

As a result of the quantitative differences between the various types of detection levels, “non-detected” compounds pose two questions: (1) Is the compound really present?, and (2) If so, at what concentration? The first question is generally hard to answer, and is dependent mainly on the analytical resources available. For the second question, the answer is “somewhere between true zero and the quantitation level applied.” For samples obtained during the trial burn that report compounds at below the detection limit, earlier U.S. EPA

(1994i) guidance has recommended that emission rates for non-detects be developed using one-half of the "detection limit" and applied in conducting the risk assessment. However, which detection limit should be used has not been explicitly defined or presented in quantitative terms.

To increase consistency and reproducibility in dealing with non-detects, U.S. EPA OSW recommends application of the MDL-derived RDL to quantify non-detects for COPCs analyzed with non-isotope dilution methods, and application of the method-defined EDL to quantify non-detects for COPCs analyzed with isotope dilution methods. Procedures for these applications are as follows:

Non-isotope Dilution Methods: Non-detects for COPCs analyzed with non-isotope dilution methods should be quantified for use in the risk assessment using an MDL-derived RDL. Commonly used non-isotope dilution methods include SW-846 Method 8260 (volatiles), SW-846 Method 8270 (semivolatiles),

1. Require the laboratory to report the actual MDL for every non-detect compound analyzed, in addition to the commonly used reporting limit, such as an EDL, EQL, or PQL. The MDL should be derived in a manner consistent with 40 CFR Part 136 Appendix B. This would also apply for analysis of each individual component of multiple component samples (e.g., front half rinse, XAD resin, condensate, Tenax tube).

   Note: Laboratories typically produce MDLs specific to each non-isotope dilution method performed by the laboratory on an annual basis.

2. Calculate an MDL-derived RDL for each COPC non-detect for quantitative application in the risk assessment. This would be obtained by multiplying the MDL, as reported by the laboratory, times 2.623 (interim factor) (U.S. EPA 1995i).

3. Adjust the RDL, as appropriate, to account for sample-specific volumetric treatments (e.g., splits and dilutions) that differ from those utilized in the Part 136 MDL determinations.

Isotope Dilution Methods (SW-846 Methods 8290,1624, 1625; and CARB 429, etc.): Non-detects for COPCs analyzed with isotope dilution methods should be quantified for use in the risk assessment using the EDL as defined by the analytical method without the use of empirical factors or other mathematical manipulations specific to the laboratory (e.g., EDL as defined in SW-846). Commonly used isotope dilution methods include SW-846 Methods 8290, 1624, and 1625.

It should be noted that the MDL definition used in 40 CFR Part 136 (see Section 2.4.1) addresses errors of the first type, false negatives. The 99 percent confidence limit stating that the MDL has only a 1 percent chance the detects will be misidentified as negative, when the compound of concern was present. Errors of the second type, false positives are not addressed. By not addressing false positives, or errors of the second type, the statistically defined default value become 50 percent. In other words, where 40 CFR did not

address false positives, the system required that 50 percent of the detects at the MDL would be false positives. This is a very conservative approach, and biased toward not missing any compounds of potential concern that may be present. The use of the MDL-derived RDL, and to a lesser extent the EDL, somewhat indirectly addresses the false positive issue. As described in defining the RDL (see Section 2.4.1), by the time the standard deviation has been multiplied by 8, the possibility of false positives is usually less than 1 percent.

2.4.3 Statistical Distribution Techniques

Many statistical distribution techniques are available for calculating a range of standard deviations to quantify non-detect concentrations of COPCs. These include random replacement scenarios, such as: (1) the uniform fill-in (UFI) method, in which each LOD value is replaced with a randomly generated data point by using a uniform distribution; (2) the log fill-in LFI method which is the same as UFI, except for using a logarithmic distribution; (3) the normal fill-in (NFI) method which is the same as UFI, except for using a log-normal distribution; and (4) the maximum likelihood estimation (MLE) techniques (Cohen and Ryan 1989; Rao et al. 1991). If determined to be applicable by the permitting authority, a Monte Carlo simulation may also be used to determine a "statistical" value for each non-detect concentration.

2.4.4 U.S. EPA OSW-Recommendations on Quantifying Non-Detects

Use of non-detects in risk assessments is dependent on the analytical method used to produce the data. In most cases, U.S. EPA will estimate emission rates for undetected COPCs (see Section 2.3) by assuming that COPCs are present at a concentration equivalent to the MDL-derived RDL for non-isotope dilution methods, or the method-defined EDL for isotope dilution methods. U.S. EPA OSW believes that these methods are reasonable and conservative, and that they represent a scientifically sound approach that allows maximum protection of the environment while recognizing the uncertainty associated with analytical measurements at very low concentrations in a real world sample matrix. It is also recognized that there are subjective components and limitations to each of the non-detect methodologies presented in this and previous guidance, including the recommended methods.

Some state permitting authorities have expressed the desire to obtain and use non-routine data (e.g., uncensored data) of defensible quality in the risk assessment as a way to deal with non-detect issues.

While this guidance does not address what forms or how such data may be used, the decision to use non-routine data in a risk assessment is not precluded just because it is different; nor does this guidance automatically approve the use of non-routine data. A permitting authority that chooses to use non-routine data should carefully identify and evaluate the limitations associated with non-routine data and clearly document this discussion in the uncertainty section of the risk assessment report.

For collection of data to be used in a risk assessment, U.S. EPA OSW recommends comprehensive sampling using typical sampling and analytical methods for VOCs, SVOCs, metals, PCDDs, PCDFs, total organics, and other appropriate constituents as necessary based on the type of waste that will be burned by the unit. A pretrial burn risk assessment can help to ensure that the desired quantitation limit (and, therefore, DREs and COPC stack gas emission rates) will be achieved during the trial burn test.

2.4.5 Estimated Maximum Possible Concentration (EMPC)

The EMPC, as defined in SW-846 Methods 8280A and 8290, is in most cases only used with the isotope dilution methods as stated. An EMPC is calculated for dioxin isomers that are characterized by a response with a signal to noise ratio of at least 2.5 for both the quantitation ions, and meet all the relevant identification criteria specified in the method, except the ion abundance ratio. Ion abundance ratios are affected by co-eluting interferences that contribute to the quantitative ion signals. As a result, one or both of the quantitative ions signals may possess positive biases.

An EMPC is a worst case estimate of the concentration. An EMPC is not a detection limit and should not be treated as a detection limit in the risk assessment. U.S. EPA OSW recommends that EMPC values be used as detections without any further manipulation (e.g., dividing by 2). However, because EMPCs are worst case estimates of stack gas concentrations, permitting authorities and facilities should consider techniques to minimize EMPCs when reporting trial and risk burn results, especially when the EMPC values result in risk estimates above regulatory levels of concern. Some techniques that may be applied to minimize EMPCs include performing additional cleanup procedures (as defined by the analytical method) on the sample or archived extract, and/or reanalyzing the sample under different chromatographic conditions.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Actual MDLs for all non-detect results
- Description of the method applied to quantify the concentration of non-detects

2.5 CONCENTRATIONS DETECTED IN BLANKS

Blank samples are intended to provide a measure of any contamination that may have been introduced into a sample either in the field while the samples were being collected, in transport to the laboratory, or in the laboratory during sample preparation or analysis. Blank samples are analyzed in the same manner as the site samples from the trail burn. In order to prevent the inclusion of non-site related compounds in the risk assessment, the concentrations of compounds detected in blanks should be compared to concentrations detected in site samples collected during the trial burn. Four types of blanks are defined in the *Risk Assessment Guidance for Superfund* (U.S. EPA 1989e): trip blanks, field blanks, laboratory calibration blanks, and laboratory reagent of method blanks. Detailed definitions of each are provided below.

Trip Blank - A trip blank is used to indicate potential contamination due to migration of volatile organic compounds from the air on the site or in sample shipping containers, through the septum or around the lid of sampling vials, and into the sample. The blank accompanies the empty sample bottles to the field as well as with the site samples returning to the laboratory for analysis. The blank sample is not opened until it is analyzed in the lab with the site samples, thus making the laboratory "blind" to the identity of the blanks.

Field Blank - A field blank is used to determine if field sampling or cleaning procedures (e.g., insufficient cleaning of sample equipment) result in cross-contamination of site samples. Like the trip blank, the field blank is transported to the field with empty sample bottles and is analyzed in the laboratory along with the site samples. Unlike the trip blank, however, the field blank sample is opened in the field and recovered in the same manner as the collected samples. As with trip blanks, the field blanks' containers and labels should be the same as for site samples and blind to the laboratory.

Instrument Blank - An instrument blank is distilled, deionized water injected directly into an instrument without having been treated with reagents appropriate to the analytical method used to analyze actual site samples. This type of blank is used to indicate contamination in the instrument itself.

Laboratory Reagent of Method Blank - A laboratory reagent of method blank results from the treatment of distilled, deionized water with all of the reagents and manipulations (e.g., degestions or extractions) to which site samples will be subjected. Positive results in the reagent blank may indicate either contamination of the chemical reagents or the glassware and implements used to store or prepare the sample and resulting solutions. Although a laboratory following good laboratory practices will have its analytical processed under control, in some instances method blank contaminants cannot be entirely eliminated.

Water Used for Blanks - For all the blanks described above, results are reliable only if the water comprising the blank was clean. For example, if the laboratory water comprising the trip blank was contaminated with VOCs prior to being taken to the field, then the source of VOC contamination in the trip blank cannot be isolated.

Blank data should be compared with the results with which the blanks are associated. However, if the association between blanks and data can not be made, blank data should be compared to the results from the entire sample data set.

U.S. EPA (1989e) makes a division in comparison between blanks containing common laboratory contaminants and blanks containing contaminants not commonly used in laboratories. Compounds considered to be common laboratory contaminants are acetone, 2-butanone (methyl ethyl ketone), methylene chloride, toluene, and the phthalate esters. If compounds considered to be common laboratory contaminants are detected in the blanks, then sample results are not considered to be detected unless the concentrations in the sample are equal to or exceed ten times the maximum amount detected in the applicable blanks. If the concentration of a common laboratory contaminant in a sample is less than ten times the blank concentration, then the compound is treated as a non-detect in that particular sample.

In some limited cases, it may be appropriate to consider blanks which contain compounds that are not considered by U.S. EPA to be common laboratory contaminants as identified above. In these limited cases, sample results are not considered to be detected unless the concentrations in the sample exceed five times the maximum amount detected in the applicable blanks. If the concentration in a sample is less than five times the blank concentration, then the compound is treated as a non-detect in that particular sample.

Permitting authorities should carefully consider the evaluation of blank data in the overall context of the risk assessment and permitting process. U.S. EPA OSW expects that issues related to non-laboratory contaminant blanks to be minimal because data collection and analysis efforts in support of trial and risk burns are expected to be of high quality in strict conformance to QA/QC plans and SOPs. The trial and risk

burn data should be carefully evaluated to ensure that the level of contamination present in the blanks does not compromise the integrity of the data for purposes of risk assessment, or result in retesting in order to properly address data quality issues.

When considering blank contamination in the COPC selection process, permitting authorities should ensure that:

(1) The facility or data gatherer has made every reasonable attempt to ensure good data quality and has rigorously implemented the QA/QC Plan and good industry sampling and testing practices.

(2) Trial and risk burn data has not been submitted to the permitting authority as "blank corrected." Rather, the permitting authority has the full opportunity to review the data absent additional manipulation by the data gatherer.

(3) The effect of the blank correction on the overall risk estimates, if such an effect is considered, is clearly described in the uncertainty section of the risk assessment report.

(4) The risk assessment reports emissions rates both as measured, and as blank corrected, in situations where there is a significant difference between the two values.

Chapter 3
Air Dispersion and Deposition Modeling

What's Covered in Chapter 3:

- U.S. EPA-Recommended Air Dispersion and Deposition Model
- Air Model Development
- Site-Specific Characteristics Required for Air Modeling
- Use of Unit Emission Rate
- Partitioning of Emissions
- Meteorological Data Required for Air Modeling
- Meteorological Preprocessors and Interface Programs
- ISCST3 Model Input Files
- ISCST3 Model Execution
- Use of Modeled Output
- Modeling Fugitive Emissions
- Estimating Media Concentrations

Combustion of materials produces residual amounts of pollution that may be released to the environment. Estimation of potential ecological risks associated with these releases requires knowledge of atmospheric pollutant concentrations and annual deposition rates in the areas around the combustion facility at habitat-specific scenario locations. Air concentrations and deposition rates are usually estimated by using air dispersion models. Air dispersion models are mathematical constructs that approximate the physical processes occurring in the atmosphere that directly influence the dispersion of gaseous and particulate emissions from the stack of a combustion unit. These mathematical constructs are coded into computer programs to facilitate the computational process.

This chapter provides guidance on the development and use of the standard U.S. EPA air dispersion model that U.S. EPA expects to be used in most situations—the Industrial Source Complex Short-Term

Model (ISCST3). ISCST3 requires the use of the following information for input into the model, and consideration of output file development:

- Site-specific characteristics required for air modeling (Section 3.2)
  - Surrounding terrain (Section 3.2.1)
  - Surrounding land use (Section 3.2.2)
  - Facility building characteristics (Section 3.2.3)
- Unit emission rate (Section 3.3)
- Partitioning of emissions (Section 3.4)
- Meteorological data (Section 3.5)
- Source Characteristics (Section 3.7)

ISCST3 also requires the use of several preprocessing computer programs that prepare and organize data for use in the model. Section 3.6 describes these programs. Section 3.7 describes the structure and format of the input files. Section 3.8 describes limitations to be considered in executing ISCST3. Section 3.9 describes use of the air modeling output in the risk assessment computations. Section 3.10 discusses air modeling of fugitive emissions. Section 3.11 describes how to estimate the media concentrations of COPCs in media.

If applicable, readers are encouraged to consult the air dispersion modeling chapter (Chapter 3) of the U.S. EPA OSW guidance document *Human Health Risk Assessment Protocol* (HHRAP) (U.S. EPA 1998c) before beginning the air modeling process to ensure the consideration of specific issues related to human health risk assessment. Additionally, the *Guideline on Air Quality Models* (GAQM) (U.S. EPA 1996c) is a primary reference for all US EPA and state agencies on the use of air models for regulatory purposes. The GAQM is incorporated in 40 CFR Part 51 as Appendix W. The Office of Air Quality Planning and Support (OAQPS) provides the GAQM and extensive information on air dispersion models, meteorological data, data preprocessors, user's guides, and model applicability on the Support Center for Regulatory Air Models (SCRAM) web site at address "http://www.epa.gov/scram001/index.htm". General questions regarding air modeling or information on the web site should be addressed to "atkinson.dennis@epamail.epa.gov". Specific questions on the use of this guidance should be addressed to the appropriate permitting authority.

3.1 DEVELOPMENT OF AIR MODELS

This section (1) briefly describes the history of air model development, (2) introduces some data preprocessing programs developed to aid in preparing air model input files (these preprocessing programs are described in more detail in Sections 3.2.4 and 3.6, and (3) introduces ExInter Version 1.0, a preprocessor to ISCST3.

3.1.1 History of Risk Assessment Air Dispersion Models

Before 1990, several air dispersion models were used by U.S. EPA and the regulated community. These models were inadequate for use in risk assessments because they considered only concentration, and not the deposition of contaminants to land. The original U.S. EPA guidance (1990a) on completing risk assessments identified two models that were explicitly formulated to account for the effects of deposition.

- COMPLEX terrain model, version 1 (COMPLEX I), from which a new model—COMPLEX terrain model with DEPosition (COMPDEP)—resulted
- Rough Terrain Diffusion Model (RTDM), from which a new model—RTDMDEP—resulted

COMPDEP was updated to include building wake effects from a version of the ISCST model in use at the time. Subsequent U.S. EPA guidance (1993h; 1994b) recommended the use of COMPDEP for air deposition modeling. U.S. EPA (1993h) specified COMPDEP Version 93252, and U.S. EPA (1994b) specified COMPDEP Version 93340. When these recommendations were made, a combined ISC-COMPDEP model (a merger of the ISCST2 and COMPLEX I model) was still under development. The merged model became known as ISCSTDFT. U.S. EPA guidance (1994l) recommended the use of the ISCSTDFT model. After reviews and adjustments, this model was released as ISCST3. The ISCST3 model contains algorithms for dispersion in simple, intermediate, and complex terrain; dry deposition; wet deposition; and plume depletion.

The use of the COMPDEP, RTDMDEP, and ISCST models is described in more detail in the following user's manuals; however, all models except the current version of ISCST3 are obsolete:

- Environmental Research and Technology (ERT). 1987. *User's Guide to the Rough Terrain Diffusion Model Revision 3.20*. ERT Document P-D535-585. Concord, Massachusetts.

- Turner, D.B. 1986. *Fortran Computer Code/User's Guide for COMPLEX I Version 86064: An Air Quality Dispersion Model in Section 4. Additional Models for Regulatory Use.* Source File 31 Contained in UNAMAP (Version 6). National Technical Information Service (NTIS) PB86-222361/AS.

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- U.S. EPA. 1995c. *User's Guide for the Industrial Source Complex (ISC3) Dispersion Models, Volumes I and II.* Office of Air Quality Planning and Standards. Emissions, Monitoring, and Analysis Division. Research Triangle Park, North Carolina. EPA 454/B-95/003a. September.

Users of this document are advised that a draft version of ISCST3 that includes algorithms for estimating the dry gas deposition (currently referred to as the "Draft Dry Gas Deposition Model: GDISCDFT, Version 96248") is available on the SCRAM web site. Use of this version to support site specific air modeling applications is not required, because many of the parameters needed to execute the model are not available in guidance or the technical literature. Therefore, until the draft version is reviewed and approved, and the data is provided by U.S. EPA or in the technical literature, U.S. EPA OSW recommends that the current version of ISCST3, in conjunction with the procedure presented in this guidance (Appendix B) for estimating dry gas deposition using deposition velocity and gas concentration, should be used for risk assessments.

3.1.2 Preprocessing Programs

ISCST3 requires the use of additional computer programs, referred to as "preprocessing" programs. These programs manipulate available information regarding surrounding buildings and meteorological data into a format that can be used by ISCST3. Currently, these programs include the following:

- PCRAMMET (Personal Computer Version of the Meteorological Preprocessor for the old RAM program) prepares meteorological data for use in ISCST3. The program organizes data—such as precipitation, wind speed, and wind direction—into rows and columns of information that are read by ISCST3. The PCRAMMET User's Guide contains detailed information for preparing the required meteorological input file for the ISCST3 model (U.S. EPA 1995b).

- Building Profile Input Program (BPIP) calculates the maximum crosswind widths of buildings, which ISCST3 then uses to estimate the effects on air dispersion. This effect on dispersion by surrounding buildings is typically known as building downwash or wake effects. The BPIP User's Guide contains detailed information for preparing the required building dimensions (length, height, and width) and locations for the ISCST3 model (U.S. EPA 1995d).

- Meteorological Processor for Regulatory Models (MPRM) prepares meteorological data for use in the ISCST3 by using on-site meteorological data rather than data from government sources (National Weather Service [NWS] or the Solar And Meteorological Surface Observational Network [SAMSON]). MPRM merges on-site measurements of precipitation, wind speed, and wind direction with off-site data from government sources into rows and columns of information that are read by ISCST3. The MPRM User's Guide contains information for preparing the required meteorological input file for the ISCST3 model (U.S. EPA 1996e).

Most air dispersion modeling performed to support risk assessments will use PCRAMMET and BPIP. MPRM will generally not be used unless on-site meteorological information is available. However, only MPRM is currently scheduled to be updated to include the meteorological parameters (solar radiation and leaf area index) required to execute the dry deposition of vapor algorithms included in the new version of ISCST3. The draft version of MPRM is available for review and comment on the SCRAM web site as GDMPRDFT (dated 96248).

3.1.3 Expert Interface (ExInter Version 1.0)

ExInter is an expert interface system enhanced by U.S. EPA Region 6 for the ISCST3 model. By enhancing ExInter, the goal of U.S. EPA Region 6 was to support the in-house performance of air dispersion modeling by regional U.S. EPA and state agency personnel at hazardous waste combustion units necessary to support risk assessments conducted at these facilities. ExInter enables the user to build input files and run ISCST3 and its preprocessor programs in a Windows-based environment. Specific procedures for developing input files are stored in an available knowledge database. The underlying premise of the ExInter system is that the knowledge of an "expert" modeler is available to "nonexpert" modeling personnel at all times. However, some air modeling experience is required to use ExInter and its components as recommended in this guidance. The ExInter program has been written in Microsoft Visual C++ in a Microsoft Windows environment.

ExInter allows for a generic source category that comprises point, area, and volume sources. For each source type, the program queries the relevant variables for the user. In addition to asking about the inputs regarding the source types, ExInter also asks about control options, receptors, meteorology, and output formats. ExInter then creates an input file, as required by the ISCST3 dispersion model. ExInter also allows the user to run the ISCST3 model and browse the results file.

Version 1.0 of ExInter provides for input parameters to model dry gas deposition included in a draft version of ISCST3. However, the data required for dry gas deposition requires a literature search and prior regulatory approval. The procedure presented in this guidance (Appendix B) for estimating dry gas deposition using deposition velocity and gas concentration is appropriate without prior approval. More detailed information on how to use ExInter can be found in the following:

- U.S. EPA. 1996i. *User's Guide for ExInter 1.0. Draft Version.* U.S. EPA Region 6 Multimedia Planning and Permitting Division. Center for Combustion Science and Engineering. Dallas, Texas. EPA/R6-096-0004. October.

ExInter is available on the SCRAM web site at "http://www.epa.gov/scram001/index.htm" under the Modeling Support section "Topics for Review". Six self-extracting compressed files contain all components for installation and use. The user's guide is accessed interactively using the help command. Individual user's guides to ISCST3, BPIP, PCRAMMET, and MPRM also provide good references for

using ExInter components. ExInter requires a minimum of 15 megabytes of free hard disk space, Windows 3.1, 8 megabytes of system memory, and a 486 processor.

3.2 SITE-SPECIFIC INFORMATION REQUIRED TO SUPPORT AIR MODELING

Site-specific information for the facility and surrounding area required to support air dispersion modeling includes (1) the elevation of the surrounding land surface or terrain, (2) surrounding land uses, and (3) characteristics of on-site buildings that may affect the dispersion of COPCs into the surrounding environment.

Often, site-specific information required to support air dispersion modeling can be obtained from review of available maps and other graphical data on the area surrounding the facility. The first step in the air modeling process is a review of available maps and other graphical data on the surrounding area. U.S. Geological Survey (USGS) 7.5-minute topographic maps (1:24,000) extending to 10 kilometers from the facility, and USGS 1:250,000 maps extending out to 50 kilometers, should be obtained to identify site location, nearby terrain features, waterbodies and watersheds, ecosystems, special ecological habitats, and land use. Aerial photographs are frequently available for supplemental depiction of the area. An accurate facility plot plan—showing buildings, stacks, property and fence lines—is also needed. Facility information including stack and fugitive source locations, building corners, plant property, and fence lines should be provided in Universal Transverse Mercator (UTM) grid coordinates in meters east and north in both USGS reference systems.

Most USGS paper 7.5-minute topographic maps are published in the North American Datum system established in 1927 (NAD 27). However, most digital elevation data (e.g., USGS Digital Elevation Mapping) is in the 1983 revised system (NAD 83). Special consideration should be given not to mix source data obtained from USGS maps based on NAD 27 with digital terrain elevation data based on NAD 83. Emission source information should be obtained in the original units from the facility data, and converted to metric units for air modeling, if necessary. Digital terrain data can be acquired from USGS or another documented source.

The specific information that must be collected is described in the following subsections. Entry of this information into the ISCST3 input files is described in Section 3.7.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- All site-specific maps, photographs, or figures used in developing the air modeling approach
- Mapped identification of facility information including stack and fugitive source locations, locations of facility buildings surrounding the emission sources, and property boundaries of the facility

3.2.1 Surrounding Terrain Information

Terrain is important to air modeling because air concentrations and deposition rates are greatly influenced by the height of the plume above local ground level. Terrain is characterized by elevation relative to stack height. For air modeling purposes, terrain is referred to as "complex" if the elevation of the surrounding land within the assessment area—typically defined as anywhere within 50 kilometers from the stack—is above the top of the stack evaluated in the air modeling analysis. Terrain at or below stack top is referred to as "simple." ISCST3 implements U.S. EPA guidance on the proper application of air modeling methods in all terrain if the modeler includes terrain elevation for each receptor grid node and specifies the appropriate control parameters in the input file.

Even small terrain features may have a large impact on the air dispersion and deposition modeling results and, ultimately, on the risk estimates. U.S. EPA OSW recommends that most air modeling include terrain elevations for every receptor grid node. Some exceptions may be those sites characterized by very flat terrain where the permitting authority has sufficient experience to comfortably defer the use of terrain data because its historical effect on air modeling results has been shown to be minimal.

In addition to maps which are used to orient and facilitate air modeling decisions, the digital terrain data used to extract receptor grid node elevations should be provided in electronic form. One method of obtaining receptor grid node elevations is using digital terrain data available from the USGS on the Internet at web site "http://www.usgs.gov". An acceptable degree of accuracy is provided by the USGS "One Degree" (e.g., 90 meter data) data available as "DEM 250" 1:250,000 scale for the entire United States free of charge. USGS 30-meter data is available for a fee. Either 90-meter or 30-meter data is sufficient for most risk assessments which utilize 100 meter or greater grid spacing. Digital terrain data may also be purchased from a variety of commercial vendors which may require vendor-provided programs to extract

the data. The elevations may also be extracted manually at each receptor grid node from USGS topographic maps.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Description of the terrain data used for air dispersion modeling
- Summary of any assumptions made regarding terrain data
- Description of the source of any terrain data used, including any procedures used to manipulate terrain data for use in air dispersion modeling

3.2.2 Surrounding Land Use Information

Land use information in the risk assessment is used for purposes of air dispersion modeling and the identification or selection of exposure scenario locations (see Chapter 4) in the risk assessment. Land use analysis for purposes of selecting exposure scenario locations usually occurs out to a radius of 50 kilometers from the centroid of the stacks to ensure identification of all receptors that may be impacted. However, in most cases, air modeling performed out to a radius of 10 kilometers allows adequate characterization for the evaluation of exposure scenario locations. If a facility with multiple stacks or emission sources is being evaluated, the radius should be extended from the centroid of a polygon drawn from the various stack coordinates.

Land use information is also important to air dispersion modeling, but at a radius closer (3 kilometers) to the emission source(s). Certain land uses, as defined by air modeling guidance, effect the selection of air dispersion modeling variables. These variables are known as dispersion coefficients and surface roughness. USGS 7.5-minute topographic maps, aerial photographs, or visual surveys of the area typically are used to define the air dispersion modeling land uses (www.usgs.gov).

3.2.2.1 Land Use for Dispersion Coefficients

The Auer method specified in the Guideline on Air Quality Models (40 CFR Part 51, Appendix W) is used to define land use for purposes of specifying the appropriate dispersion coefficients built into ISCST3.

Land use categories of "rural" or "urban" are taken from the methods of Auer (Auer 1978). Areas typically defined as rural include residences with grass lawns and trees, large estates, metropolitan parks and golf courses, agricultural areas, undeveloped land, and water surfaces. Auer typically defines an area as "urban" if it has less than 35 percent vegetation coverage or the area falls into one of the following use types:

Urban Land Use		
Type	**Use and Structures**	**Vegetation**
I1	Heavy industrial	Less than 5 percent
I2	Light/moderate industrial	Less than 5 percent
C1	Commercial	Less than 15 percent
R2	Dense single/multi-family	Less than 30 percent
R3	Multi-family, two-story	Less than 35 percent

In general, the Auer method is described as follows:

Step 1 Draw a radius of 3 kilometers from the center of the stack(s) on the site map.

Step 2 Inspect the maps, and define in broad terms whether the area within the radius is rural or urban, according to Auer's definition.

Step 3 Classify smaller areas within the radius as either rural or urban, based on Auer's definition. (It may be prudent to overlay a grid [for example, 100 by 100 meters] and identify each square as primarily rural or urban)

Step 4 Count the total of rural squares; if more than 50 percent of the total squares are rural, the area is rural; otherwise, the area is urban.

Alternatively, digital land use databases may be used in a computer-aided drafting system to perform this analysis.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Description of the methods used to determine land use surrounding the facility
- Copies of any maps, photographs, or figures used to determine land use
- Description of the source of any computer-based maps used to determine land use

3.2.2.2 Land Use for Surface Roughness Height (Length)

Surface roughness height—also referred to as (aerodynamic) surface roughness length—is the height above the ground at which the wind speed goes to zero. Surface roughness affects the height above local ground level that a particle moves from the ambient air flow above the ground (for example in the plume) into a "captured" deposition region near the ground. That is, ISCST3 causes particles to be "thrown" to the ground at some point above the actual land surface, based on surface roughness height. Surface roughness height is defined by individual elements on the landscape, such as trees and buildings.

U.S. EPA (1995b) recommended that land use within 5 kilometers of the stack be used to define the average surface roughness height. For consistency with the method for determining land use for dispersion coefficients (Section 3.2.2.1), the land use within 3 kilometers generally is acceptable for determination of surface roughness. Surface roughness height values for various land use types are as follows:

Surface Roughness Heights for Land Use Types and Seasons (meters)				
Land Use Type	**Spring**	**Summer**	**Autumn**	**Winter**
Water surface	0.0001	0.0001	0.0001	0.0001
Deciduous forest	1.00	1.30	0.80	0.50
Coniferous forest	1.30	1.30	1.30	1.30
Swamp	0.20	0.20	0.20	0.05
Cultivated land	0.03	0.20	0.05	0.01
Grassland	0.05	0.10	0.01	0.001
Urban	1.00	1.00	1.00	1.00
Desert shrubland	0.30	0.30	0.30	0.15

Source: Sheih, Wesley, and Hicks (1979)

If a significant number of buildings are located in the area, higher surface roughness heights (such as those for trees) may be appropriate (U.S. EPA 1995b). A specific methodology for determining average surface roughness height has not been proposed in prior guidance documents. For facilities using National Weather Service surface meteorological data, the surface roughness height for the measurement site may be set to 0.10 meters (grassland, summer) without prior approval. If a different value is proposed for the measurement site, the value should be determined applying the following procedure to land use at the measurement site. For the application site, the following method should be used to determine surface roughness height:

Step 1 Draw a radius of 3 kilometers from the center of the stack(s) on the site map.

Step 2 Inspect the maps, and use professional judgment to classify the areas within the radius according to the PCRAMMET categories (for example water, grassland, cultivated land, and forest); a site visit may be necessary to verify some classifications.

Step 3 Calculate the wind rose directions from the 5 years of meteorological data to be used for the study (see Section 3.4.1.1); a wind rose can be prepared and plotted by using the U.S. EPA WRPLOT program from the U.S. EPA's Support Center for Regulatory Air Models bulletin board system (SCRAM BBS).

Step 4 Divide the circular area into 16 sectors of 22.5 degrees, corresponding to the wind rose directions (for example, north, north-northeast, northeast, and east-northeast) to be used for the study.

Step 5 Identify a representative surface roughness height for each sector, based on an area-weighted average of the land use within the sector, by using the land use categories identified above.

Step 6 Calculate the site surface roughness height by computing an average surface roughness height weighted with the frequency of wind direction occurrence for each sector.

Alternative methods of determining surface roughness height may be proposed for agency approval prior to use in an air modeling analysis.

3.2.3 Information on Facility Building Characteristics

Building wake effects have a significant impact on the concentration and deposition of COPCs near the stack. Building wake effects are flow lines that cause plumes to be forced down to the ground much sooner than they would if the building was not there. Therefore, the ISCST3 model contains algorithms for

evaluating this phenomenon, which is also referred to as "building downwash." The downwash analysis should consider all nearby structures with heights at least 40 percent of the height of the shortest stack to be modeled. The 40 percent value is based on Good Engineering Practice (GEP) stack height of 2.5 times the height of nearby structures or buildings (stack height divided by 2.5 is equal to 0.40 multiplied by the stack height [40 CFR Part 51 Appendix W]). Building dimensions and locations are used with stack heights and locations in BPIP to identify the potential for building downwash. BPIP and the BPIP user's guide can be downloaded from the SCRAM web site and should be referred to when addressing specific questions. The BPIP output file is in a format that can be copied and pasted into the source (SO) pathway of the ISCST3 input file. The following procedure should be used to identify buildings for input to BPIP:

Step 1 Lay out facility plot plan, with buildings and stack locations clearly identified (building heights must be identified for each building); for buildings with more than one height or roof line, identify each height (BPIP refers to each height as a tier).

Step 2 Identify the buildings required to be included in the BPIP analysis by comparing building heights to stack heights. The building height test requires that only buildings at least 40 percent of the height of a potentially affected stack be included in the BPIP input file. For example, if a combustion unit stack is 50 feet high, only buildings at least 20 feet (0.40 multiplied by 50 feet) tall will affect air flow at stack top. Any buildings shorter than 20 feet should not be included in the BPIP analysis. The building height test is performed for each stack and each building.

Step 3 Use the building distance test to check each building required to be included in BPIP from the building height test. For the building distance test, only buildings "nearby" the stack will affect air flow at stack top. "Nearby" is defined as "five times the lesser of building height or crosswind width" (U.S. EPA 1995d). A simplified distance test may be used by considering only the building height rather than the crosswind width. While some buildings with more height than width will be included unnecessarily using this simplification, BPIP will identify correctly only the building dimensions required for ISCST3.

As an example, if a plot plan identifies a 25-foot tall building that is 115 feet from the 50-foot tall combustion unit stack center to the closest building corner. The building distance test, for this building only, is five times the building height, or 125 feet (five multiplied by the building height, 25 feet). This building would be included in the BPIP analysis, because it passes the building height test and building distance test.

Step 4 Repeat steps 2 and 3 for each building and each stack, identifying all buildings to be included in the BPIP. If the number of buildings exceeds the BPIP limit of eight buildings, consider combining buildings, modifying BPIP code for more buildings, or using third-party commercial software which implements BPIP. If two buildings are closer than the height of the taller building, the two buildings may be combined. For example, two buildings are 40 feet apart at their closest points. One building is 25 feet high, and the

other building is 50 feet high. The buildings could be combined into one building for input to BPIP. For input to BPIP, the corners of the combined building are the outer corners of the two buildings. For unusually shaped buildings with more than the eight corners allowed by BPIP, approximate the building by using the eight corners that best represent the extreme corners of the building. The BPIP User's Guide contains additional description and illustrations on combining buildings, and BPIP model limitations (U.S. EPA 1995d).

Step 5 Mark off the facility plot plan with UTM grid lines. Extract the UTM coordinates of each building corner and each stack center to be included in BPIP input file. Although BPIP allows the use of "plant coordinates," U.S. EPA OSW requires that all inputs to the air modeling be prepared using UTM coordinates (meters) for consistency. UTM coordinates are rectilinear, oriented to true north, and in metric units required for ISCST3 modeling. Almost all air modeling will require the use of USGS topographic data (digital and maps) for receptor elevations, terrain grid files, location of plant property, and identification of surrounding site features. Therefore, using an absolute coordinate system will enable the modeler to check inputs at each step of the analysis. Also, the meteorological data are oriented to true north. Significant errors will result from ISCST3 if incorrect stack or building locations are used, plant north is incorrectly rotated to true north, or incorrect base elevations are used. With computer run times of multiple years of meteorological data requiring many hours (up to 40 hours for one deposition run with depletion), verification of locations at each step of preparing model inputs will prevent the need to remodel.

Several precautions and guidelines should be observed in preparing input files for BPIP:

- Before BPIP is run, the correct locations should be graphically confirmed. One method is to plot the buildings and stack locations by using a graphics program. Several commercial programs incorporating BPIP provide graphic displays of BPIP inputs.
- U.S. EPA OSW recommends, in addition to using UTM coordinates for stack locations and building corners, using meters as the units for height.
- Carefully include the stack base elevation and building base elevations by using the BPIP User's Guide instructions.
- Note that the BPIP User's Guide (revised February 8, 1995) has an error on page 3-5, Table 3-1, under the "TIER(i,j)" description, which incorrectly identifies tier height as base elevation.
- BPIP mixes the use of "real" and "integer" values in the input file. To prevent possible errors in the input file, note that integers are used where a count is requested (for example, the number of buildings, number of tiers, number of corners, or number of stacks).
- The stack identifications (up to eight characters) in BPIP must be identical to those used in the ISCST3 input file, or ISCST3 will report errors.

For most sites, BPIP executes in less than 1 minute. The array of 36 building heights and 36 building widths (one for each of 36 10-degree direction sectors) are input into the ISCST3 input file by cutting and pasting from the BPIP output file. The five blank spaces preceding "SO" in the BPIP output file must be deleted so that the "SO" begins in the first column of the ISCST3 input file.

One use of BPIP is to design stack heights for new facilities or determine stack height increases required to avoid the building influence on air flow, which may cause high concentrations and deposition near the facility. The output for BPIP provides the GEP heights for stacks. Significant decreases in concentrations and deposition rates will begin at stack heights at least 1.2 times the building height, and further decreases occur at 1.5 times building height, with continual decreases of up to 2.5 times building height (GEP stack height) where the building no longer influences stack gas.

3.3 USE OF UNIT EMISSION RATE

The ISCST3 model is usually run with a unit emission rate of 1.0 g/s in order to preclude having to run the model for each specific COPC. The unitized concentration and deposition output from ISCST3, using a unit emission rate, are adjusted to the COPC-specific air concentrations and deposition rates in the estimating media concentration equations (see Section 3-11) by using COPC-specific emission rates obtained during the trial burn (see Chapter 2). Concentration and deposition are directly proportional to a unit emission rate used in the ISCST3 modeling.

For facilities with multiple stacks or emission sources, each source must be modeled separately. The key to not allowing more than one stack in a single run is the inability to estimate stack-specific risks, which limits the ability of a permitting agency to evaluate which stack is responsible for the resulting risks. Such ambiguity would make it impossible for the agency to specify protective, combustion unit-specific permit limits. If a facility has two or more stacks with identical characteristics (emissions, stack parameters, and nearby locations), agency approval may be requested to represent the stacks with a single set of model runs.

3.4 PARTITIONING OF EMISSIONS

COPC emissions to the environment occur in either vapor or particle phase. In general, most metals and organic COPCs with very low volatility (refer to fraction of COPC in vapor phase [*Fv*] less than 0.05, as

presented in Appendix A-2) are assumed to occur only in the particle phase. Organic COPCs occur as either only vapor phase (refer to *Fv* of 1.0, as presented in Appendix A-2) or with a portion of the vapor condensed onto the surface of particulates (e.g., particle-bound). COPCs released only as particulates are modeled with different mass fractions allocated to each particle size than the mass fractions for the organics released in both the vapor and particle-bound phases. Due to the limitations of the ISCST3 model, estimates of vapor phase COPCs, particle phase COPCs, and particle-bound COPCs cannot be provided in a single pass (run) of the model. Multiple runs are required. An example of this requirement is the risk assessment for the WTI incinerator located in East Liverpool, Ohio. The study used three runs; a vapor phase run for organic COPCs, a particle run with mass weighting of the particle phase metals and organic COPCs with very low volatility, and a particle run with surface area weighting of the particle-bound organic COPCs .

3.4.1 Vapor Phase Modeling

ISCST3 output for vapor phase air modeling runs are vapor phase ambient air concentration and wet vapor deposition at receptor grid nodes based on the unit emission rate. Vapor phase runs do not require a particle size distribution in the ISCST3 input file. One vapor phase run is required for each receptor grid that is modeled (see Section 3.7).

3.4.2 Particle Phase Modeling (Mass Weighting)

ISCST3 uses algorithms to compute the rate at which dry and wet removal processes deposit particulate-phase COPCs emitted from a combustion unit stack to the Earth's surface. Particle size is the main determinant of the fate of particles in air flow, whether dry or wet. The key to dry particle deposition rate is the terminal, or falling, velocity of a particle. Particle terminal velocity is calculated mainly from the particle size and particle density. Large particles fall more rapidly than small particles and are deposited closer to the stack. Small particles have low terminal velocities, with very small particles remaining suspended in the air flow. Wet particle deposition also depends on particle size as larger particles are more easily removed, or scavenged, by falling liquid (rain) or frozen (snow or sleet) precipitation. An ISCST3 modeling analysis of particle phase emissions for deposition rate requires an initial estimate of the particle size distribution, distinguished on the basis of particle diameter.

The diameters of small particulates contained in stack emissions are usually measured in micrometers. The distribution of particulate by particle diameter will differ from one combustion process to another, and is greatly dependent on (1) the type of furnace, (2) the design of the combustion chamber, (3) the composition of the feed fuel, (4) the particulate removal efficiency, (5) the design of the APCS, (6) the amount of air, in excess of stoichiometric amounts, that is used to sustain combustion, and (7) the temperature of combustion. However, based on these variables, the particle size distribution cannot be calculated, but only directly measured or inferred from prior data. Unfortunately, few studies have been performed to directly measure particle size distributions from a variety of stationary combustion sources (U.S. EPA 1986a).

U.S. EPA OSW recommends that existing facilities perform stack tests to identify particle size distribution. These data should represent actual operating conditions for the combustion unit and air pollution control device (APCD) that remove particulate from the stack gas. A table of particle size distribution data should be prepared using stack test data in the format in Table 3-1.

U.S. EPA OSW expects that stack test data will be different from the values presented in Table 3-1 because of the use of particle "cut size" for the different cascade impactor filters (or Coulter counter-based distributions) used during actual stack sampling. The test method will drive the range of particle sizes that are presented in the results of the stack test. However, because ISCST3 requires mean particle diameter for each particle size distribution, and the stack test data identifies only the mass ("weight") of particles in a range bounded by two specific diameters, stack test data must be converted into a mean particle diameter which approximates the diameter of all the particles within a defined range. Consistent with U.S. EPA 1993h, the mean particle diameter is calculated by using the following equation:

$$D_{mean} = [0.25 \cdot (D_1^3 + D_1^2 D_2 + D_1 D_2^2 + D_2^3)]^{0.33} \qquad \text{Equation 3-1}$$

where

D_{mean} = Mean particle diameter for the particle size category (μm)
D_1 = Lower bound cut of the particle size category (μm)
D_2 = Upper bound cut of the particle size category (μm)

For example, the mean particle diameter of 5.5 μm in Table 3-1 is calculated from a lower bound cut size (assuming a cascade impactor is used to collect the sample) of 5.0 μm to an upper bound cut size of 6.15 μm. In this example, the mean particle diameter is calculated as:

$$D_{mean} = \left[0.25\ (5.0^3 + (5.0)^2(6.15) + (5.0)(6.15)^2 + 6.15^3)\right]^{0.33} = 5.5\ \mu m$$

TABLE 3-1

GENERALIZED PARTICLE SIZE DISTRIBUTION, AND PROPORTION OF AVAILABLE SURFACE AREA, TO BE USED AS A DEFAULT IN DEPOSITION MODELING IF SITE-SPECIFIC DATA ARE UNAVAILABLE

1	2	3	4	5	6
Mean Particle Diameter [a] (μm)	**Particle Radius (μm)**	**Surface Area/ Volume (μm^{-1})**	**Fraction of Total Mass[b]**	**Proportion Available Surface Area**	**Fraction of Total Surface Area**
> 15.0	7.50	0.400	0.128	0.0512	0.0149
12.5	6.25	0.480	0.105	0.0504	0.0146
8.1	4.05	0.741	0.104	0.0771	0.0224
5.5	2.75	1.091	0.073	0.0796	0.0231
3.6	1.80	1.667	0.103	0.1717	0.0499
2.0	1.00	3.000	0.105	0.3150	0.0915
1.1	0.55	5.455	0.082	0.4473	0.1290
0.7	0.40	7.500	0.076	0.5700	0.1656
< 0.7	0.40	7.500	0.224	1.6800	0.4880

Notes:

a Geometric mean diameter in a distribution from U.S. EPA (1980a), as presented in U.S. EPA (1993h)
b The terms mass and weight are used interchangeably when using stack test data

From Table 3-1, the mean particle diameter is 5.5 μm. The mass of particulate from the 5.0 μm stack test data is then assigned to the 5.5 μm mean particle diameter for the purpose of computing the "fraction of total mass."

Typically, eight to ten mean particle diameters are available from stack test results. As determined from a sensitivity analysis conducted by The Air Group-Dallas under contract to U.S. EPA Region 6 (www.epa.gov/region06), a minimum of three particle size categories (> 10 microns, 2-10 microns, and < 2 microns) detected during stack testing are generally the most sensitive to air modeling with ISCST-3 (U.S. EPA 1997). For facilities with stack test results which indicate mass amounts lower than the detectable limit (or the filter weight is less after sampling than before), a single mean particle size diameter of 1.0 microns should be used to represent all mass (e.g., particle diameter of 1.0 microns or a particle mass fraction of 1.0) in the particle and particle-bound model runs. Because rudimentary methods for stack testing may not detect the very small size or amounts of COPCs in the particle phase, the use of a 1.0 micron particle size will allow these small particles to be included properly as particles in the risk assessment exposure pathways while dispersing and depositing in the air model similar in behavior to a vapor.

After calculating the mean particle diameter (Column 1), the fraction of total mass (Column 4) per mean particle size diameter must be computed from the stack test results. For each mean particle diameter, the stack test data provides an associated mass of particulate. The fraction of total mass for each mean particle diameter is calculated by dividing the associated mass of particulate for that diameter by the total mass of particulate in the sample. In many cases, the fractions of total mass will not sum to 1.0 due to rounding errors. In these instances, U.S. EPA OSW advocates that the remaining mass fraction be added into the largest mean particle diameter mass fraction to force the total mass to 1.0.

Direct measurements of particle-size distributions at a proposed new facility may be unavailable, so it will be necessary to provide assumed particle distributions for use in ISCST3. In such instances, a representative distribution may be used. The unit on which the representative distribution is based should be as similar as practicable to the proposed unit. For example, the default distribution provided in Table 3-1 is not appropriate for a hazardous waste burning boiler with no APCD or a wet scrubber, because it is based on data from different type of unit. However, the generalized particle size (diameter) distribution in Table 3-1 may be used as a default for some combustion facilities equipped with either ESPs

or fabric filters, because the distribution is relatively typical of particle size arrays that have been measured at the outlet to advanced equipment designs (Buonicore and Davis 1992; U.S. EPA 1986a; U.S. EPA 1987a).

After developing the particulate size distribution based on mass, this distribution is used in ISCST3 to apportion the mass of particle phase COPCs (metals and organics with F_v values less than 0.05) based on particle size. Column 4 of Table 3-1 (as developed from actual stack test data) is used in the ISCST3 input file to perform a particulate run with the particle phase COPCs apportioned based on mass weighting.

3.4.3 Particle-Bound Modeling (Surface Area Weighting)

A surface area weighting, instead of mass weighting, of the particles is used in separate particle runs of ISCST3. Surface area weighting approximates the situation where a semivolatile organic contaminant that has been volatilized in the high temperature environment of a combustion system and then condensed to the surface of particles entrained in the combustion gas after it cools in the stack. Thus, the apportionment of emissions by particle diameter becomes a function of the surface area of the particle that is available for chemical adsorption (U.S. EPA 1993h).

The first step in apportioning COPC emissions by surface area is to calculate the proportion of available surface area of the particles. If particle density is held constant (such as 1 g/m^3), the proportion of available surface area of aerodynamic spherical particles is the ratio of surface area (*S*) to volume (*V*), as follows:

- Assume aerodynamic spherical particles.
- Specific surface area of a spherical particle with a radius, r—$S = 4 \pi r^2$
- Volume of a spherical particle with a radius, r—$V = 4/3 \pi r^3$
- Ratio of *S* to *V*—$S/V = 4 \pi r^2 / (4/3 \pi r^3) = 3/r$

The following uses the particle size distribution in Table 3-1 as an example of apportioning the emission rate of the particle-bound portion of the COPC based on surface area. This procedure can be followed for apportioning actual emissions to the actual particle size distribution measured at the stack. In Table 3-1, a

spherical particle having a diameter of 15 μm (Column 1) has a radius of 7.5 μm (Column 2). The proportion of available surface area (assuming particle density is constant) is 0.400 (S/V = 3/7.5), which is the value in Column 3. Column 4 shows that particles with a mean diameter of 15 μm, constitute 12.8 percent of the total mass. Multiplication of Column 3 by Column 4 yields a value in Column 5 of 0.0512. This value is an approximation of the relative proportion of total surface area, based on the percent of particles that are 15 μm in diameter. The sum of Column 5 yields the total surface area of all particles in the particle size distribution. In this example, the sum is 3.4423. Column 6 is the fraction of total surface area represented by the specific particle diameter in the distribution, and is calculated by dividing the relative proportion of surface area (Column 5) for a specific diameter by the total relative proportion of surface area (3.4423 square micrometers [μm^2]). In the example of the 15 μm-diameter particle, the fraction of total surface area available for adsorption is 0.0149 (0.0512/3.4423). This procedure is then repeated for all particle sizes in the array.

After developing the particulate size distribution based on surface area, this distribution is used in ISCST3 to apportion mass of particle-bound COPCs (most organics) based on particle size. Column 6 of Table 3-1 (as developed from actual stack test data) is used in the ISCST3 input file to perform a particulate run for the particle-bound COPCs apportioned based on surface area weighting.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Copies of all stack test data used to determine particle size distribution
- Copies of all calculations made to determine particle size distribution, fraction of total mass, and fraction of total surface area

3.5 METEOROLOGICAL DATA

To model air concentration and deposition, the ISCST3 model requires a variety of meteorological information:

1. Air concentration
    a. Hourly values

(1) Wind direction (degrees from true north)
(2) Wind speed (m/s)
(3) Dry bulb (ambient air) temperature (K)
(4) Opaque cloud cover (tenths)
(5) Cloud ceiling height (m)

b. Daily values

(1) Morning mixing height (m)
(2) Afternoon mixing height (m)

2. Deposition

a. Dry particle deposition—hourly values for surface pressure (millibars)

b. Wet particle deposition—hourly values
(1) Precipitation amount (inches)
(2) Precipitation type (liquid or frozen)

c. Dry vapor deposition (when available)—hourly values for solar radiation (watts/m^2)

As shown in Figure 3-1, these data are available from several different sources. For most air modeling, five years of data from a representative National Weather Service station is recommended. However, in some instances where the closest NWS data is clearly not representative of site specific meteorlogical conditions, and there is insufficient time to collect 5 years of onsite data, 1 year of onsite meteorological data (consistent with GAQM) may be used to complete the risk assessment. The permitting authority should approve the representative meteorological data prior to performing air modeling.

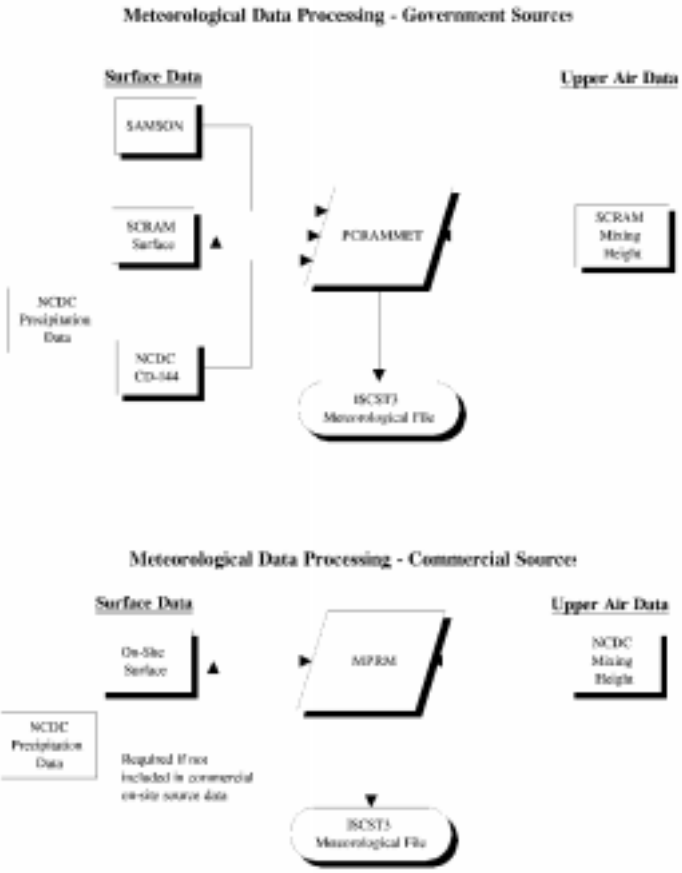
The following subsections describe how to select the surface and upper air data that will be used in conjunction with the ISCST3 model. Section 3.7 describes the computer programs used to process the meteorological data for input to the ISCST3 model.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Identification of all sources of meteorological data

FIGURE 3-1

SOURCES OF METEOROLOGICAL DATA



3.5.1 Surface Data

Surface data can be obtained from SAMSON in CD-ROM format. SAMSON data are available for 239 airports across the U.S. for the period of 1961 through 1990. The National Climate Data Center (NCDC) recently released the update to SAMSON through 1995 surface data. However, since the upper air (mixing height) data available from the U.S. EPA SCRAM web site has not been updated to cover this recent data period, it is acceptable to select the representative 5 years of meteorological data from the period up through 1990. SAMSON data contain all of the required input parameters for concentration, dry and wet particle deposition, and wet vapor deposition. SAMSON also includes the total solar radiation data required for dry vapor deposition, which may be added to ISCST3 in the future. Alternatively, some meteorological files necessary for running ISCST3 are also available on the SCRAM BBS for NWS stations located throughout the country (SCRAM BBS is part of the Office of Air Quality and Planning and Standards Technology Transfer Network [OAQPS TTN]). The meteorological data, preprocessors, and user's guides are also located on the SCRAM web site at "http://www.epa.gov/scram001/index.htm". However, these files do not contain surface pressure, types of precipitation (present weather), or precipitation amount. Although the ISCST3 model is not very sensitive to surface pressure variations, and a default value may be used, precipitation types and amounts are necessary for air modeling wet deposition. Precipitation data are available from the National Climatic Data Center (NCDC), and are processed by PCRAMMET to supplement the SCRAM BBS surface data. NCDC also has surface data in CD-144 format, which contains all of the surface data, including precipitation.

The SAMSON CD-ROM for the eastern, central, or western (Volumes I, II, and III) United States may be purchased from NCDC in Asheville, North Carolina.

National Climatic Data Center **Federal Building** **37 Battery Park Avenue** **Asheville, NC 28801-2733** **Customer Service: (704) 271-4871**	
File type:	File name:
Hourly precipitation amounts	NCDC TC-3240
Hourly surface observations with precipitation type	NCDC TD-3280
Hourly surface observations with precipitation type	NCDC SAMSON CD-ROM (Vol. I, II, and/or III)
Twice daily mixing heights from nearest station	NCDC TD-9689 (also available on SCRAM web site for 1984 through 1991)

PCRAMMET and MPRM are the U.S. EPA meteorological preprocessor programs for preparing the surface and upper air data into a meteorlogical file of hourly parameters for input into the ISCST3 model. Most air modeling analyses will use PCRAMMET to process the National Weather Service data. However, both preprocessors require the modeler to replace any missing data. Before running PCRAMMET or MPRM, the air modeler must fill in missing data to complete 1 full year of values. A procedure recommended by U.S. EPA for filling missing surface and mixing height data is documented on the SCRAM BBS under the meteorological data section. If long periods of data are missing, and these data are not addressed by the U.S. EPA procedures on the SCRAM BBS, then a method must be developed for filling in missing data. One option is to fill the time periods with "surrogate place holder" data in the correct format with correct sequential times to complete preparation of the meteorological file. Place holder data are typically considered the last valid hourly data of record. Then, when ISCST3 is running, the `MSGPRO` keyword in the COntrol pathway can be used to specify that data are missing. Note that the `DEFAULT` keyword must not be used with `MSGPRO`. Since the missing data keyword is not approved generally for regulatory air modeling, the appropriate agency must provide approval prior to use. All processing of meteorological data should be completely documented to include sources of data, decision criteria for selection, consideration for precipitation amounts, preprocessor options selected, and filled missing data.

The most recently available 5 years of complete meteorological data contained on SAMSON, or more recent sources, should be used for the air modeling. It is desirable, but not mandatory, that the 5 years are

consecutive. The use of less than five years of meteorological data should be approved by appropriate authorities. The following subsections describe important characteristics of the surface data.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Electronic copy of the ISCST3 input code used to enter meteorological information
- Description of the selection criteria and process used to identify representative years used for meteorological data
- Identification of the 5 years of meteorological selected
- Summary of the procedures used to compensate for any missing data

3.5.1.1 Wind Speed and Wind Direction

Wind speed and direction are two of the most critical parameters in ISCST3. The wind direction promotes higher concentration and deposition if it persists from one direction for long periods during a year. A predominantly south wind, such as on the Gulf Coast, will contribute to high concentrations and depositions north of the facility. Wind speed is inversely proportional to concentration in the ISCST3 algorithms. The higher the wind speed, the lower will be the concentration. If wind speed doubles, the concentration and deposition will be reduced by one-half. ISCST3 needs wind speed and wind direction at the stack top. Most air modeling is performed using government sources of surface data. Wind data are typically measured at 10 meters height at NWS stations. However, since some stations have wind speed recorded at a different height, the anemometer height must always be verified so that the correct value can be input into the PCRAMMET meteorological data preprocessing program. ISCST3 assumes that wind direction at stack height is the same as measured at the NWS station height. ISCST3 uses a wind speed profile to calculate wind speed at stack top. This calculation exponentially increases the measured wind speed from the measured height to a calculated wind speed at stack height (U.S. EPA 1995d).

3.5.1.2 Dry Bulb Temperature

Dry bulb temperature, or ambient air temperature, is the same temperature reported on the television and radio stations across the country each day. It is measured at 2 meters above ground level. Air temperature

is used in ISCST3 in the buoyant plume rise equations developed by Briggs (U.S. EPA 1995c). The model results are not very sensitive to air temperature, except at extremes. However, buoyant plume rise is very sensitive to the stack gas temperature. Buoyant plume rise is mainly a result of the difference between stack gas temperature and ambient air temperature. Conceptually, it is similar to a hot air balloon. The higher the stack gas temperature, the higher will be the plume rise. High plume heights result in low concentrations and depositions as the COPCs travel further and are diluted in a larger volume of ambient air before reaching the surface. The temperature is measured in K, so a stack gas temperature of 450°F is equal to 505 K. Ambient temperature of 90°F is equal to 305 K, and 32°F is 273 K. A large variation in ambient temperature will affect buoyant plume rise, but not as much as variations in stack gas temperature.

3.5.1.3 Opaque Cloud Cover

PCRAMMET uses opaque cloud cover to calculate the stability of the atmosphere. Stability determines the dispersion, or dilution, rate of the COPCs. Rapid dilution occurs in unstable air because of surface heating that overturns the air. With clear skies during the day, the sun heats the Earth's surface, thereby causing unstable air and dilution of the stack gas emission stream. Stable air results in very little mixing, or dilution, of the emitted COPCs. A cool surface occurs at night because of radiative loss of heat on clear nights. With a cloud cover, surface heating during the day and heat loss at night are reduced, resulting in moderate mixing rates, or neutral stability. Opaque cloud cover is a measure of the transparency of the clouds. For example, a completely overcast sky with 10/10ths cloud cover may have only 1/10th opaque cloud cover if the clouds are high, translucent clouds that do not prevent sunlight from reaching the Earth's surface. The opaque cloud cover is observed at NWS stations each hour.

3.5.1.4 Cloud Ceiling Height

Cloud height is required in PCRAMMET to calculate stability. Specifically, the height of the cloud cover affects the heat balance at the Earth's surface. Cloud ceiling height is measured or observed at all NWS stations provided on the SAMSON CD-Roms and the U.S. EPA SCRAM web site.

3.5.1.5 Surface Pressure

Surface pressure is required by ISCST3 for calculating dry particle deposition. However, ISCST3 is not very sensitive to surface pressure. SAMSON and NCDC CD-144 data include surface pressure. SCRAM BBS surface data do not include surface pressure. U.S. EPA believes that, if SCRAM BBS surface data are used, a default value of 1,000 millibars can be assumed, with little impact on modeled results.

3.5.1.6 Precipitation Amount and Type

The importance of precipitation to ISCST3 results was discussed in the selection of the meteorological data period (see Section 3.5.1). Precipitation is measured at 3 feet (1 meter) above ground level. Precipitation amount and type are required to be processed by PCRAMMET or MPRM into the ISCST3 meteorological file to calculate wet deposition of vapor and particles. The amount of precipitation, or precipitation rate, will directly influence the amount of wet deposition at a specific location. Particles and vapor are both captured by falling precipitation, known as precipitation scavenging. Scavenging coefficients are required as inputs to ISCST3 for vapors with a rate specified for liquid and frozen precipitation. The precipitation type in a weather report in SAMSON or CD-144 data file will identify to ISCST3 which event is occurring for appropriate use of the scavenging coefficients entered (see Section 3.7.2.6). SCRAM BBS surface data do not include precipitation data. Supplemental precipitation files from NCDC may be read into PCRAMMET for integration into the ISCST3 meteorological file.

3.5.1.7 Solar Radiation (Future Use for Dry Vapor Deposition)

The current version of ISCST3 does not use solar radiation. Several U.S. EPA models, including the Acid Deposition and Oxidant Model (ADOM), incorporate algorithms for dry vapor deposition. At such time as U.S. EPA approves the draft version of ISCST3 which includes dry gas deposition, the hourly total solar radiation will be required. Solar radiation affects the respiratory activity of leaf surfaces, which affects the rate of vapor deposition. With a leaf area index identified in the ISCST3 input file in the future, the model will be able to calculate dry vapor deposition.

3.5.2 Upper Air Data

Upper air data, also referred to as mixing height data, are required to run the ISCST3 model. ISCST3 requires estimates of morning and afternoon (twice daily) mixing heights. PCRAMMET and MPRM use these estimates to calculate an hourly mixing height by using interpolation methods (U.S. EPA 1996e). The mixing height files are typically available for the years 1984 through 1991 on the U.S. EPA SCRAM web site. U.S. EPA OSW recommends that only years with complete mixing height data be used as input for air modeling. In some instances, data may need to be obtained from more than one station to complete five years of data. The selection of representative data should be discussed with appropriate authorities prior to performing air modeling.

Mixing height data for years prior to 1983, in addition to current mixing height data, may be purchased from NCDC as described in Section 3.5.1. The years selected for upper air data must match the years selected for surface data. If matching years of mixing height data are not available from a single upper air station, another upper air station should be used for completing the five years.

3.6 METEOROLOGICAL PREPROCESSORS AND INTERFACE PROGRAMS

After the appropriate surface and upper air data is selected following the procedures outlined in Section 3.5, additional data manipulation is necessary before the data is used with the ISCST3 model. The following subsections describe the meteorological preprocessors and interface programs used for these manipulation tasks. To eliminate any need to repeat air modeling activities, U.S. EPA OSW recommends that the selection of representative mixing height and surface data be approved by the appropriate regulatory agency before preprocessing or air modeling is conducted. Permitting authority approval also is recommended in the selection of site-specific parameter values required as input to the meteorological data preprocessors.

3.6.1 PCRAMMET

U.S. EPA OSW recommends preparing a meteorological file for ISCST3 that can be used to calculate any concentration or deposition. By preparing a file that PCRAMMET terms a “WET DEPOSITION” file, all required parameters will be available to ISCST3 for any subsequent concentration or deposition modeling.

For example, if only the concentration option is selected in ISCST3 for a specific run, ISCST3 will ignore the precipitation values in the meteorological file. For subsequent air deposition modeling, ISCST3 will access the precipitation data from the same preprocessed meteorological file.

PCRAMMET may use SAMSON, SCRAM web site, and NCDC CD-144 surface data files. U.S. EPA OSW recommends using the SAMSON option in PCRAMMET to process the SAMSON surface data and U.S. EPA SCRAM web site mixing height data. The PCRAMMET User's Guide in the table "Wet Deposition, SAMSON Data" (U.S. EPA 1995b) identifies the PCRAMMET input requirements for creating an ASCII meteorological file for running ISCST3 to calculate air concentration, and wet and dry deposition. The meteorological file created for ISCST3 will contain all of the parameters needed for air modeling of concentration and deposition.

PCRAMMET requires the following input parameters representative of the measurement site:

- Monin-Obukhov length
- Anemometer height
- Surface roughness height (at measurement site)
- Surface roughness height (at application site)
- Noon-time albedo
- Bowen ratio
- Anthropogenic heat flux
- Fraction of net radiation absorbed at surface

The PCRAMMET User's Guide contains detailed information for preparing the required meteorological input file for the ISCST3 model (U.S. EPA 1995b). The parameters listed are briefly described in the following subsections. These data are not included in the surface or mixing height data files obtained from the U.S. EPA or NCDC. Representative values specific to the site to be modeled should be carefully selected using the tables in the PCRAMMET User's Guide or reference literature. The selected values should be approved prior to processing the meteorological data.

3.6.1.1 Monin-Obukhov Length

The Monin-Obukhov length (*L*) is a measure of atmospheric stability. It is negative during the day, when surface heating causes unstable air. It is positive at night, when the surface is cooled with a stable atmosphere. In urban areas during stable conditions, the estimated value of *L* may not adequately reflect the less stable atmosphere associated with the mechanical mixing generated by buildings or structures. However, PCRAMMET requires an input for minimum urban Monin-Obukhov length, even if the area to be analyzed by ISCST3 is rural. A nonzero value for *L* must be entered to prevent PCRAMMET from generating an error message. A value of 2.0 meter for *L* should be used when the land use surrounding the site is rural (see Section 3.2.2.1). For urban areas, Hanna and Chang (1991) suggest that a minimum value of *L* be set for stable hours to simulate building-induced instability. The following are general examples of *L* values for various land use classifications:

Land Use Classification	Minimum *L*
Agricultural (open)	2 meters
Residential	25 meters
Compact residential/industrial	50 meters
Commercial (19 to 40-story buildings)	100 meters
Commercial (>40-story buildings)	150 meters

PCRAMMET will use the minimum *L* value for calculating urban stability parameters. These urban values will be ignored by ISCST3 during the air modeling analyses for rural sites.

3.6.1.2 Anemometer Height

The height of the wind speed measurements is required by ISCST3 to calculate wind speed at stack top. The wind sensor (anemometer) height is identified in the station history section of the Local Climatological Data Summary available from NCDC for every National Weather Service station. Since 1980, most National Weather Service stations measure wind speed at the height of 10 meters. However, some stations operate at other heights or have valid representative data during years of operation at more than one height. The modeler must verify the correct measurement height for each year of data prior to processing with

PCRAMMET and running the ISCST3 model. ISCST3 modeled results are very sensitive to small variations in wind speed.

3.6.1.3 Surface Roughness Height at Measurement Site

Surface roughness height is a measure of the height of obstacles to wind flow. It is important in ISCST3 because it determines how close a particle must be above the ground before it is "captured" for deposition on the ground. Dramatic differences in ISCST3 calculations may result from slight variations in surface roughness. For surface meteorological data from a National Weather Station, a value of 0.10 meters for the "measurement site" typically may be used without prior approval. Surface roughness is proportional, but not equal, to the physical height of the obstacles. The table in Section 3.2.2.2 lists the roughness heights that can be used as input values. These values are based on the general land use in the vicinity of the measurement site. These values should be considered in discussions with the appropriate agency modeler prior to air modeling.

3.6.1.4 Surface Roughness Height at Application Site

Determination of surface roughness height is also required at the facility (application site) for performing PCRAMMET processing to prepare an ISCST3 meteorological file. ISCST3 model results are very sensitive to the value used in PCRAMMET for this parameter. The table in Section 3.2.2.2 is applicable to the application site. A site-specific computation of a single surface roughness value representative of the site is required using the method described in Section 3.2.2.2. The computed value of surface roughness height for the application site, along with maps or photographs illustrating land use, must be approved by the appropriate agency prior to use.

3.6.1.5 Noon-Time Albedo

"Noon-time albedo" is the fraction of the incoming solar radiation that is reflected from the ground when the sun is directly overhead. Albedo is used in calculating the hourly net heat balance at the surface for calculating hourly values of Monin-Obukhov length. PCRAMMET automatically adjusts for the variation in albedo with solar elevation angle. Experience suggests that ISCST3 modeling results are not sensitive to the value selected for this parameter. Typical albedo values are presented in Table 3-2. As shown in Table

3-2, albedo values vary from 0.10 to 0.20 on water surfaces from summer to winter. The most variability is for cultivated farmland, which varies from 0.14 during spring when land is tilled to expose dark earth, to 0.60 in winter when areas are snow-covered.

Based on the information in Table 3-2, albedos are estimated to vary in rural areas from 0.14 to 0.20 for cultivated land, and from 0.18 to 0.20 for grassland. For urban areas, the variation without snow is from 0.14 to 0.18. For practical purposes, the selection of a single value for noon-time albedo to process a complete year of meteorological data is desirable. For example, the single value of 0.18 may be appropriate to process all meteorological data for an urban site. For rural sites, a single albedo value of 0.18 representative of grassland and cultivated land may be appropriate for areas without significant snow cover during winter months. For desert shrubland, a single value of 0.28 may be appropriate. A single value of 0.12 could be representative of forested areas. The permitting authority should review proposed values used in the processing of the meteorological data.

TABLE 3-2

ALBEDO OF NATURAL GROUND COVERS FOR LAND USE TYPES AND SEASONS

Land Use Type	Season[a]			
	Spring	Summer	Autumn	Winter
Water surface	0.12	0.10	0.14	0.20
Deciduous forest	0.12	0.12	0.12	0.50
Coniferous forest	0.12	0.12	0.12	0.35
Swamp	0.12	0.14	0.16	0.30
Cultivated land	0.14	0.20	0.18	0.60
Grassland	0.18	0.18	0.20	0.60
Urban	0.14	0.16	0.18	0.35
Desert shrubland	0.30	0.28	0.28	0.45

Notes:

Source—Iqbal (1983)

[a] The various seasons are defined by Iqbal (1983) as follows:

Spring: Periods when vegetation is emerging or partially green; this is a transitional situation that applies for 1 to 2 months after the last killing frost in spring.

Summer: Periods when vegetation is lush and healthy; this is typical of mid-summer, but also of other seasons in which frost is less common.

Autumn: Periods when freezing conditions are common, deciduous trees are leafless, crops are not yet planted or are already harvested (bare soil exposed), grass surfaces are brown, and no snow is present.

Winter: Periods when surfaces are covered by snow and temperatures are below freezing. Winter albedo depends on whether a snow cover is present continuously, intermittently, or seldom. Albedo ranges from about 0.30 for bare snow cover to about 0.65 for continuous cover.

3.6.1.6 Bowen Ratio

The Bowen ratio is a measure of the amount of moisture at the surface. The presence of moisture affects the heat balance resulting from evaporative cooling, which, in turn, affects the hourly Monin-Obukhov length calculated by PCRAMMET. Surface moisture is highly variable. Daytime Bowen ratios are presented in Table 3-3.

Bowen ratio values vary throughout the country. For example, in urban areas where annual rainfall is less than 20 inches, a single Bowen ratio value of 4.0 may be representative. For rural areas, a Bowen ratio value of 2.0 may be appropriate for grassland and cultivated land. For areas where annual rainfall is greater than 20 inches, U.S. EPA OSW recommends a single Bowen ratio value of 2.0 for urban areas; and 0.7 for rural forests, grasslands, and cultivated lands. The applicable permiting authority should review proposed values used in the processing of the meteorological data.

3.6.1.7 Anthropogenic Heat Flux

Anthropogenic heat is the surface heating caused by human activity, including automobiles and heating systems. It is used to calculate hourly L values (Monin-Obukhov lengths). Table 3-4 presents anthropogenic heat flux (Q_f) values that have been calculated for several urban areas around the world. In rural areas, U.S. EPA OSW recommends that a value of 0.0 Watts/m^2 be used for the Q_f. A value of 20.0 Watts/m^2 is appropriate for large urban areas based on the annual value from Table 3-4 for Los Angeles.

3.6.1.8 Fraction of Net Radiation Absorbed at the Ground

Also used for calculating hourly values of Monin-Obukhov length, fraction of net radiation absorbed at the ground is the last component of radiative heat balance. Based on the net radiation (Q_*) values presented in Table 3-4, and recommendations presented in the PCRAMMET User's Manual based on Oke (1982), U.S. EPA OSW recommends values of 0.15 for rural areas and 0.27 for urban areas (U.S. EPA 1995b).

TABLE 3-3

DAYTIME BOWEN RATIOS BY LAND USE, SEASON, AND PRECIPITATION CONDITIONS

Land Use	Season[a]			
	Spring	Summer	Autumn	Winter
Dry Conditions				
Water (fresh and salt)	0.1	0.1	0.1	2.0
Deciduous forest	1.5	0.6	2.0	2.0
Coniferous forest	1.5	0.6	1.5	2.0
Swamp	0.2	0.2	0.2	2.0
Cultivated land	1.0	1.5	2.0	2.0
Grassland	1.0	2.0	2.0	2.0
Urban	2.0	4.0	4.0	2.0
Desert shrubland	5.0	6.0	10.0	2.0
Average Conditions				
Water (fresh and salt)	0.1	0.1	0.1	1.5
Deciduous forest	0.7	0.3	1.0	1.5
Coniferous forest	0.7	0.3	0.8	1.5
Swamp	0.1	0.1	0.1	1.5
Cultivated land	0.3	0.5	0.7	1.5
Grassland	0.4	0.8	1.0	1.5
Urban	1.0	2.0	2.0	1.5
Desert shrubland	3.0	4.0	6.0	6.0

TABLE 3-3

DAYTIME BOWEN RATIO BY LAND USE, SEASON, AND PRECIPITATION CONDITIONS (Continued)

Land Use	Season[a]			
	Spring	Summer	Autumn	Winter
Wet Conditions				
Water (fresh and salt)	0.1	0.1	0.1	0.3
Deciduous forest	0.3	0.2	0.4	0.5
Coniferous forest	0.3	0.2	0.3	0.3
Swamp	0.1	0.1	0.1	0.5
Cultivated land	0.2	0.3	0.4	0.5
Grassland	0.3	0.4	0.5	0.5
Urban	0.5	1.0	1.0	0.5
Desert shrubland	1.0	5.0	2.0	2.0

Note:

Source—Paine (1987)

[a] The various seasons are defined by Iqbal (1983) as follows:

Spring: Periods when vegetation is emerging or partially green; this is a transitional situation that applies for 1 to 2 months after the last killing frost in spring.

Summer: Periods when vegetation is lush and healthy; this is typical of mid-summer, but also of other seasons in which frost is less common.

Autumn: Periods when freezing conditions are common, deciduous trees are leafless, crops are not yet planted or are already harvested (bare soil exposed), grass surfaces are brown, and no snow is present

Winter: Periods when surfaces are covered by snow and temperatures are below freezing.

TABLE 3-4

ANTHROPOGENIC HEAT FLUX (Q_f) AND NET RADIATION (Q_*) FOR SEVERAL URBAN AREAS

Urban Area (Latitude)	Population (Millions)	Population Density (Persons/km^2)	Per Capita Energy Use (MJ x 10^3/year)	Q_f (Watts/m^2) (Season)	Q_* (Watts/m^2)
Manhattan (40° North)	1.7	28,810	128	117 (Annual) 40 (Summer) 198 (Winter)	93 (Annual)
Montreal (45° North)	1.1	14,102	221	99 (Annual) 57 (Summer) 153 (Winter)	52 (Annual) 92 (Summer) 13 (Winter)
Budapest (47° North)	1.3	11,500	118	43 (Annual) 32 (Summer) 51 (Winter)	46 (Annual) 100 (Summer) -8 (Winter)
Sheffield (53° North)	0.5	10,420	58	19 (Annual)	56 (Annual)
West Berlin (52° North)	2.3	9,830	67	21 (Annual)	57 (Annual)
Vancouver (49° North)	0.6	5,360	112	19 (Annual) 15 (Summer) 23 (Winter)	57 (Annual) 107 (Summer) 6 (Winter)
Hong Kong (22° North)	3.9	3,730	34	4 (Annual)	110 (Annual)
Singapore (1° North)	2.1	3,700	25	3 (Annual)	110 (Annual)
Los Angeles (34° North)	7.0	2,000	331	21 (Annual)	108 (Annual)
Fairbanks (64° North)	0.03	810	740	19 (Annual)	18 (Annual)

Note:

Source—Oke (1978)

3.6.2 MPRM

For on-site data, a new version of MPRM is used to mesh on-site data with NWS data in the preparation of the meteorological input file. MPRM performs the same meteorological file preparation as PCRAMMET, except the source of the surface data in MPRM consists of on-site measurements (U.S. EPA 1996e). MPRM includes extensive QA/QC for values that are out of range. MPRM also checks for missing data and summarizes values that require editing to fill missing data. After a complete surface file passes the quality checks, it is processed with NCDC mixing height data. NCDC data are purchased to correspond to the collection period of the on-site surface data. Mixing height data available on SCRAM's web site ends in 1991. A delay of about 3 months can occur for obtaining mixing height data from NCDC to process with recent on-site surface data.

Inputs to MPRM for preparing an ISCST3 meteorological file for concentration and deposition are the same as for PCRAMMET. Section 3.6.1 provides methods for determining values for these parameters.

Draft versions of ISCST3 and MPRM are available for review which implement dry vapor deposition. These versions are GDISCDFT (dated 96248) and GDMPRDFT (dated 96248), respectively. They may be found on the U.S. EPA SCRAM web site under "Topics for Review". These draft models are not the current regulatory versions and should not be used without approval from the appropriate permitting authority.

3.7 ISCST3 MODEL INPUT FILES

A thorough instruction of how to prepare the input files for ISCST3 is presented in the ISC3 User's Guide, Volume I (U.S. EPA 1995c), which is available for downloading from the SCRAM BBS. The example ISCST3 input file is provided in Figure 3-2 from the air dispersion modeling chapter (Chapter 3) of the U.S. EPA HHRAP (U.S. EPA 1998). This example illustrates a single year run (1984), for particle phase COPC emissions from a single stack, to compute acute (1-hour average) and chronic (annual average) and provide single year results in one hour and annual average plot files for post-processing. For ecological risk assessments, only the annual average air parameters are required, not the 1-hour values. However, by modeling both the 1-hour and annual averages in a single set of runs, the ISCST3 air dispersion model will

provide the necessary air parameters for use in both the human health and ecological risk assessments. The specification of a terrain grid file in the TG pathway is optional. Each air modeling analysis has unique issues and concerns that should be addressed in the risk assessment report. U.S. EPA OSW recommends that the air modeling methodology be consistent in data collection, model set-up, and model output. This consistency will assist both the modeler and U.S. EPA in communicating and interpreting model results. The risk assessment report should document each section of the ISCST3 input file to identify consistent methods.

Three sets of ISCST3 runs are required for each COPC emission source. As discussed in Section 3.4, separate ISCST3 runs are required to model vapor phase COPCs, particle phase COPCs, and particle-bound phase COPCs for each source (stack or fugitive) of COPCs. The ISCST3 "Control Secondary Keywords" used for these three runs are:

Vapor Phase:	`CONC WDEP`
Particle Phase:	`CONC DDEP WDEP DEPOS`
Particle-Bound Phase:	`CONC DDEP WDEP DEPOS`

For ISCST3 modeling to provide air parameters for ecological risk assessments, only the total deposition (DEPOS) of the particle and particle-bound phases are required. The control secondary keywords for concentration in the air (CONC) and the components of deposition to the ground, dry deposition (DDEP) and wet deposition (WDEP), are not required to be output separately by ISCST3. However, by specifying these control secondary keywords as illustrated, the ISCST3 model will compute the needed air parameters for both human health and ecological risk assessments. ISCST3 requires site-specific inputs for source parameters, receptor locations, meteorological data, and terrain features. The model is prepared for

execution by creating an input file. The input file is structured in five (or six if a terrain grid file is used) sections, or pathways, designated by two-letter abbreviations:

ISCST3 INPUT FILE SECTIONS	
Section	**Abbreviation**
Control	CO
Source	SO
Receptor	RE
Meteorology	ME
Terrain Grid (Optional)	*TG*
Output	OU

The following subsections describe how to specify the parameters for each pathway in the ISCST3 input file.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Electronic and hard copies of ISCST3 input file for all air modeling runs

3.7.1 COntrol Pathway

Model options (MODELOPT) are specified in the COntrol pathway to direct ISCST3 in the types of computations to perform. U.S. EPA OSW recommends that air modeling specify the DFAULT parameter to use the following regulatory default options:

- Use stack-tip downwash (except for Schulman-Scire downwash).
- Use buoyancy-induced dispersion (except for Schulman-Scire downwash).
- Do not use final plume rise (except for building downwash).
- Use the calms processing routines.

- Use upper-bound concentration estimates for sources influenced by building downwash from super-squat buildings.
- Use default wind speed profile exponents.
- Use default vertical potential temperature gradients.

The CONC parameter specifies calculation of air concentrations for vapor and particles. The DDEP and WDEP parameters specify dry and wet deposition. The DEPOS specifies computation of total (wet and dry) deposition flux. Since ISCST3 currently does not include an algorithm for the dry deposition of vapor phase COPCs, only wet deposition is specified for vapor phase runs. Note that dry deposition of vapor phase is addressed in the pathway equations during the risk assessment using the concentration of the vapor phase and a deposition velocity. DRYDPLT and WETDPLT are used for plume depletion resulting from dry and wet removal. U.S. EPA OSW recommends the following command lines for each of the three runs (these are for rural areas; substitute URBAN for urban areas):

Vapor:
```
CO MODELOPT DFAULT CONC WDEP WETDPLT RURAL
```

Particle Phase:
```
CO MODELOPT DFAULT CONC DDEP WDEP DEPOS DRYDPLT WETDPLT
RURAL
```

Particle-Bound:
```
CO MODELOPT DFAULT CONC DDEP WDEP DEPOS DRYDPLT WETDPLT
RURAL
```

Note that only the total deposition (DEPOS) air parameter values are required for the ecological risk assessment pathways. The modeler may elect not to include CONC, DDEP and WDEP as separate output components from ISCST3 if the air modeling results will not be used for a human health risk assessment. However, the control secondary keywords must always be specified for plume depletion through the dry deposition (DRYDPLT) and wet deposition (WETDPLT) processes.

FIGURE 3-2

EXAMPLE INPUT FILE FOR "PARTICLE PHASE"

```
CO STARTING
CO TITLEONE Example input file, particle phase run
CO TITLETWO 1984 met data, Baton Rouge Surface, Boothville Upper Air
CO MODELOPT DFAULT CONC DDEP WDEP DEPOS DRYDPLT WETDPLT RURAL
CO AVERTIME 1 ANNUAL
CO POLLUTID UNITY
CO TERRHGTS ELEV
CO RUNORNOT RUN
CO SAVEFILE 84SAVE1 5 84SAVE2
** Restart incomplete runs with INITFILE, changing '**' to 'CO'
** INITFILE 84SAVE1
CO FINISHED

SO STARTING
SO LOCATION STACK1 POINT 637524. 567789. 347.
SO SRCPARAM STACK1 1.0 23.0 447.0 14.7 1.9
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29
SO BUILDWID STACK1 14.02 15.51 16.53 17.05 17.05 16.53 15.51 14.03
SO BUILDWID STACK1 12.10 14.02 15.51 16.53 17.05 17.05 16.53 15.51
SO BUILDWID STACK1 14.02 12.10 14.02 15.51 16.53 17.05 17.05 16.53
SO BUILDWID STACK1 15.51 14.02 12.10 14.02 15.51 16.53 17.05 17.05
SO BUILDWID STACK1 16.53 15.51 14.02 12.10
SO PARTDIAM STACK1 0.35 0.70 1.10 2.00 3.60 5.50 8.10 12.5 15.0
SO MASSFRAX STACK1 0.22 0.08 0.08 0.11 0.10 0.07 0.10 0.11 0.13
SO PARTDENS STACK1 1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
SO PARTSLIQ STACK1 7E-5 5E-5 6E-5 1.3E-4 2.6E-4 3.9E-4 5.2E-4 6.7E-4 6.7E-4
SO PARTSICE STACK1 2E-5 2E-5 2E-5   4E-5   9E-5 1.3E-4 1.7E-4 2.2E-4 2.2E-4
SO SRCGROUP ALL
SO FINISHED

RE STARTING
RE ELEVUNIT METERS
RE DISCCART 630000. 565000. 352.
RE DISCCART 630500. 565000. 365.
RE DISCCART 631000. 565000. 402.
      ...
      (ARRAY OF DISCRETE RECEPTORS)
      ...
RE DISCCART 635000. 570000. 387.
RE FINISHED

ME STARTING
ME INPUTFIL 84BTR.WET
ME ANEMHGHT 10.0
ME SURFDATA 13970 1984 BATON_ROUGE
ME UAIRDATA 12884 1984 BOOTHVILLE
ME FINISHED

TG STARTING
TG INPUTFIL TERRAIN.TER
TG LOCATION 0.0 0.0
TG ELEVUNIT METERS
TG FINISHED

OU STARTING
OU RECTABLE ALLAVE FIRST
OU PLOTFILE 1 ALL FIRST BTR841.PLT
OU PLOTFILE ANNUAL ALL BTR84A.PLT
OU FINISHED
```

For each of the three runs for each emission source, 5 years of off-site (e.g., National Weather Service from SAMSON) meteorological data are completed. For sites with meteorological data collected on-site, the appropriate permitting authority should be notified for the data period required for a risk assessment. The averaging times (AVERTIME) should be specified as 'ANNUAL' to compute long-term (annual average) ecological risk. Optionally, the '1' may be specified for convenience in modeling for the maximum 1-hour averages used in computing acute human health risks. Each phase run may be repeated five times (one for each year, or a total of 15 ISCST3 runs) to complete a set of 15 runs for the full five years of meteorological data.

Alternatively, the modeler may combine the 5 years of meteorological data into a single meteorological data file and complete only 3 runs for each emission source (one run for each phase). Section 3.5.1.1 of the ISC3 User's Guide (U.S. EPA 1995c), includes a complete discussion of combining multiple years of meteorological data into a single file prior to running ISCST3. The modeler should select the 'ANNUAL' averaging time for all risk assessment runs, regardless of the number of years in the meteorological data file. The incorrect selection of 'PERIOD' will not compute the correct deposition rates required by the risk assessment equations (refer to Section 3.2.3 of the ISC3 User Guide, Volume I). No additional ISCST3 model execution time is required to obtain 1-year or 5-year air modeling values.

In addition, ISCST3 allows the specification of COPC half-life and decay coefficients. Unless approved by the permitting authority with documentation of COPC-specific data, these keywords should not be used when conducting air modeling to support risk assessments. The TERRHGTS keyword with the ELEV parameter typically should be used to model terrain elevations at receptor grid nodes. The FLAGPOLE keyword specifies receptor grid nodes above local ground level and is not typically used for most air modeling to perform impacts at ground level.

U.S. EPA OSW also recommends that SAVEFIL be used to restart ISCST3 in the event of a computer or power failure during long runs. SAVEFIL is best used by specifying two save files, each with a different name. The save interval should be no longer than 5 days for large runs. If two save files are used, and a

failure occurs during writing to the savefile, no more than 10 days will be lost. The INITFILE command should be used to restart the runs after the failure, as shown in the following example:

```
CO SAVEFILE SAVE1 5 SAVE2
** INITFILE SAVE1
```

ISCST3 will save the results alternately to SAVE1 and SAVE2 every 5 days. If the run fails after successfully writing to SAVE1, the ISCST3 run can be restarted by replacing the two asterisks (*) in the INITFILE line with CO and running ISCST3 again. The run will begin after the last day in SAVE1. The modeler should change the names of the save files (e.g., SAVE3 and SAVE4) in the 'CO SAVEFILE' command line prior to restarting ISCST3 to avoid overwriting the SAVE1 and SAVE2 files containing valid data from the interrupted run. Note that the MULTYEAR keyword is not used for computing long-term averages and should not be specified.

The following is an example of the COntrol pathway computer code for a single-year ISCST3 particle run:

```
CO STARTING
CO TITLEONE Example input file, particle pahse run, 1 year
CO TITLETWO 1984 met data, Baton Rouge Surface, Boothville Upper Air
CO MODELOPT DFAULT CONC DDEP WDEP DEPOS DRYDPLT WETDPLT RURAL
CO AVERTIME 1 ANNUAL
CO POLLUTID UNITY
CO TERRHGTS ELEV
CO RUNORRUN RUN
CO SAVEFILE 84SAVE1 5 84SAVE2
** Restart incomplete runs with INITFILE, changing '**' to 'CO'
** INITFILE SAVE1
CO FINISHED
```

Additional runs for the other 4 years are set up with the same COntrol pathway, except for the title description and SAVEFILE filenames.

3.7.2 SOurce Pathway

As discussed in Section 3.3, ISCST3 normally uses a unit emission rate of 1.0 g/s. Additional source characteristics required by the model (typically obtained from the Part B permit application and trial burn report) include the following:

- Source type (point source for stack emissions; area or volume for fugitive emissions)
- Source location (UTM coordinates, m)
- Source base elevation
- Emission rate (1.0 g/s)
- Stack height (m)
- Stack gas temperature (K)
- Stack gas exit velocity (m/s)
- Stack inside diameter (m)
- Building heights and widths (m)
- Particle size distribution (percent)
- Particle density (g/cm^3)
- Particle and gas scavenging coefficients (unitless)

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Input values with supporting documentation for each parameter identified in Section 3.7.2

3.7.2.1 Source Location

The location keyword of the SOurce pathway (`SO LOCATION`) identifies source type, location, and base elevation. The source type for any stack is referred to as a point source in ISCST3. Fugitive source emissions are discussed in section 3.10. The source location must be entered into ISCST3. Locations should be entered in UTM coordinates. The easterly coordinate is entered to the nearest meter; for example, 637524 meters UTM-E (no commas are used). The northerly coordinate is entered to the nearest meter; for example, a northerly coordinate of 4,567,789 meters UTM-N is entered as 4567789. The base

elevation of each stack must be entered in meters. Base elevation may be obtained from a USGS topographic map, facility plot plans or USGS digital data base.

An example input for the location keyword on the SOurce pathway includes source type, location, and base elevation in the following format:

```
SO LOCATION STACK1 POINT 637524. 4567789. 347.
```

3.7.2.2 Source Parameters

The source parameters keyword of the SOurce pathway (`SO SRCPARAM`) identifies the emission rate, stack height, stack temperature, stack velocity, and stack diameter. The unit emission rate is entered as 1.0 g/s. Stack height is the height above plant base elevation on the `SO LOCATION` keyword. Stack exit temperature is the most critical stack parameter for influencing concentration and deposition. High stack temperatures result in high buoyant plume rise, which, in turn, lowers concentration and deposition rates. Stack temperatures should be based on stack sampling tests for existing stacks. For new or undefined stacks, manufacturer's data for similar equipment should be used. Stack exit velocity should be calculated from actual stack gas flow rates and stack diameter. Actual stack gas flow rates should be determined for existing stacks during stack sampling. Representative values for new or undefined sources should be obtained from manufacturer's data on similar equipment. Stack diameter is the inside diameter of the stack at exit.

Following is an example of the source parameter input in the SOurce pathway for emission rate (grams per second), stack height (meters), stack temperature (K), stack velocity (meters per second), and stack diameter (meters):

```
SO SRCPARAM STACK1 1.0 23.0 447.0 14.7 1.9
```

3.7.2.3 Building Parameters

The building height and width keywords of the SOurce pathway (`SO BUILDHGT; SO BUILDWID`) identify the building dimensions that most influence the air flow for each of the 36 10-degree directions

surrounding a stack. The dimensions are calculated by using the U.S. EPA program BPIP, as described in Section 3.2.4.

The BPIP output file is input as follows:

```
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29

SO BUILDWID STACK1 14.02 15.51 16.53 17.05 17.05 16.53 15.51 14.03
SO BUILDWID STACK1 12.10 14.02 15.51 16.53 17.05 17.05 16.53 15.51
SO BUILDWID STACK1 14.02 12.10 14.02 15.51 16.53 17.05 17.05 16.53
SO BUILDWID STACK1 15.51 14.02 12.10 14.02 15.51 16.53 17.05 17.05
SO BUILDWID STACK1 16.53 15.51 14.02 12.10
```

3.7.2.4 Particle Size Distribution

ISCST3 requires particle size distribution for determining deposition velocities. U.S. EPA OSW recommends site-specific stack test data for existing sources. New or undefined sources may use the particle size distribution presented in Table 3-1.

The following example is the ISCST3 input for particle phase run. From Table 3-1, the distribution for 9 mean diameter sizes includes the data required for the keywords of the SOurce pathway (`SO PARTDIAM; SO MASSFRAX`). The `PARTDIAM` is taken from Column 1 (Mean Particle Diameter). The `MASSFRAX` is taken from Column 4 (Fraction of Total Mass).

```
SO PARTDIAM STACK1 0.35 0.70 1.10 2.00 3.60 5.50 8.10 12.5 15.0
SO MASSFRAX STACK1 0.22 0.08 0.08 0.11 0.10 0.07 0.10 0.11 0.13
```

The example for the ISCST3 input for the particle-bound run is described below. From Table 3-1, the `PARTDIAM` is the same. The `MASSFRAX` is taken from Column 6 (Fraction of Total Surface Area).

```
SO PARTDIAM STACK1 0.35 0.70 1.10 2.00 3.60 5.50 8.10 12.5 15.0
SO MASSFRAX STACK1 0.49 0.17 0.13 0.09 0.05 0.02 0.02 0.01 0.02
```

3.7.2.5 Particle Density

Particle density is also required for modeling the air concentration and deposition rates of particles. Site-specific measured data on particle density should be determined for all existing sources when possible. For new or undefined sources requiring air modeling, a default value for particle density of 1.0 g/cm^3 may be used. Particles from combustion sources, however, may have densities that are less than 1.0 g/cm^3 (U.S. EPA 1994a), which would reduce the modeled deposition flux.

Following is an example of the particle density input in the SOurce pathway (`SO PARTDENS`) for the 9 mean particle size diameters of the previous example:

```
SO PARTDENS STACK1 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0
```

3.7.2.6 Scavenging Coefficients

Wet deposition flux is calculated within ISCST3 by multiplying a scavenging ratio by the vertically integrated concentration. The scavenging ratio is the product of a scavenging coefficient and a precipitation rate. Studies have shown that best fit values for the scavenging coefficients vary with particle size. For vapors, wet scavenging depends on the properties of the COPCs involved. However, not enough data are now available to adequately develop COPC-specific scavenging coefficients. Therefore, vapors are assumed to be scavenged at the rate of the smallest particles with behavior in the atmosphere that is assumed to be influenced more by the molecular processes that affect vapors than by the physical processes that may dominate the behavior of larger particles (U.S. EPA 1995c).

To use the wet deposition option in ISCST3, users must input scavenging coefficients for each particle size and a file that has hourly precipitation data. For wet deposition of vapors, a scavenging coefficient for a 0.1-μm particle may be input to simulate wet scavenging of very small (molecular) particles. Alternatively, site-specific measured washout data or a calculation based on Henry's Law constant may be approved by the appropriate permitting authority prior to analysis. Wet deposition results only during precipitation. Scavenging coefficients should be determined for each particle size from the best fit curve based on the work of Jindal and Heinhold (1991) presented in the ISC3 User's Guide (U.S. EPA 1995c). The curves are

limited to a maximum particle size of 10-μm, so all scavenging coefficients for particle sizes greater than or equal to 10-μm are assumed to be equal. This assumption follows research on wet scavenging of particles (Jindal and Heinhold 1991).

The ISCST3 model input also differentiates between frozen and liquid scavenging coefficients. As a conservative estimate, the frozen scavenging coefficients are assumed to be equal to the liquid scavenging coefficients (PEI and Cramer 1986). If desired, the user may input separate scavenging coefficients for frozen precipitation. Research on sulfate and nitrate data has shown that frozen precipitation scavenging coefficients are about one-third of the values of liquid precipitation (Scire, Strimaitis, and Yamartino 1990; Witby 1978).

Following is an example of the particle liquid (rain) and frozen (sleet or snow) scavenging coefficients input in the SOurce pathway for 9 mean particle size diameters assuming particles are scavenged by frozen precipitation at 1/3 the rate of liquid precipitation:

```
SO PARTSLIQ STACK1 7E-5 5E-5 6E-5 1.3E-4 2.6E-4 3.9E-4 5.2E-4 6.7E-4 6.7E-4
SO PARTSICE STACK1 2E-5 2E-5 2E-5   4E-5   9E-5 1.3E-4 1.7E-4 2.2E-4 2.2E-4
```

The complete SOurce pathway for the example particle phase input file is as follows:

```
SO STARTING
SO LOCATION STACK1 POINT 637524. 4567789. 347.
SO SRCPARAM STACK1 1.0 23.0 447.0 14.7 1.9
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29 18.29 18.29 18.29 18.29
SO BUILDHGT STACK1 18.29 18.29 18.29 18.29
SO BUILDWID STACK1 14.02 15.51 16.53 17.05 17.05 16.53 15.51 14.03
SO BUILDWID STACK1 12.10 14.02 15.51 16.53 17.05 17.05 16.53 15.51
SO BUILDWID STACK1 14.02 12.10 14.02 15.51 16.53 17.05 17.05 16.53
SO BUILDWID STACK1 15.51 14.02 12.10 14.02 15.51 16.53 17.05 17.05
SO BUILDWID STACK1 16.53 15.51 14.02 12.10
SO PARTDIAM STACK1 0.35 0.70 1.10 2.00 3.60 5.50 8.10 12.5 15.0
SO MASSFRAX STACK1 0.22 0.08 0.08 0.11 0.10 0.07 0.10 0.11 0.13
SO PARTDENS STACK1 1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0  1.0
SO PARTSLIQ STACK1 7E-5 5E-5 6E-5 1.3E-4 2.6E-4 3.9E-4 5.2E-4 6.7E-4 6.7E-4
SO PARTSICE STACK1 2E-5 2E-5 2E-5   4E-5   9E-5 1.3E-4 1.7E-4 2.2E-4 2.2E-4
SO SRCGROUP ALL
SO FINISHED
```

When modeling air vapors using ISCST3, the following is an example of the SOurce pathway input for wet vapor scavenging coefficients that replaces the PARTDIAM, MASSFRAX, PARTDENS, PARTSLIQ and PARTSICE lines in the above example:

```
SO GAS-SCAV STACK1 LIQ 1.7E-4
SO GAS-SCAV STACK1 ICE 0.6E-4
```

3.7.3 REceptor Pathway

The REceptor pathway identifies sets or arrays of receptor grid nodes identified by UTM coordinates for which ISCST3 generates estimates of air parameters including air concentration, dry and wet deposition, and total deposition. Previous U.S. EPA guidance (U.S. EPA 1994a) recommended using a polar receptor grid to identify maximum values, because polar grids provide coverage over large areas with a reduced number of receptor grid nodes, thereby reducing computer run times. However, U.S. EPA Region 6 experience indicates that, although the use of polar grids may reduce computer run times, air modelers typically choose a different option, because the benefit of reduced run time is offset by difficulties in identifying polar grid locations in absolute UTM coordinates for (1) extracting terrain values from digital terrain files, and (2) selecting receptor grid node locations for evaluation of ecosystems and special ecological habitats (see Chapter 4).

Receptor grid node arrays may be generated by using ISCST3 grid generation. However, assigning terrain elevations for each receptor grid node in an array associated with the generated grid can result in errors. One method of obtaining a Cartesian grid with terrain elevations is to open the USGS DEM file in a graphics program (e.g., SURFER®). Selection of the grid option samples the DEM file, at the user-specified spacing, over a range of east (x) and north (y) values. The specified x and y locations extract terrain elevation (z) from the DEM file at the desired receptor grid node for air modeling with the appropriate terrain elevations at each receptor grid node. These x, y, and z values are saved as a text file with one receptor grid node per line. A text editor is used to prefix each line with "`RE DISCCART`" to specify a discrete receptor grid node in ISCST3 format. Commercial receptor grid generators are also available. One commercial program (Lakes Environmental Software) generates the recommended receptor grid node array and extracts terrain elevations from the USGS DEM downloaded files, or any terrain file in x-y-z format.

The following is an example of the REceptor pathway for discrete receptor grid nodes at 500-meter spacing and including terrain elevations (in meters):

```
RE STARTING
RE ELEVUNIT METERS
RE DISCCART 630000. 565000. 352.
RE DISCCART 630500. 565000. 365.
RE DISCCART 631000. 565000. 402.
      ↓
RE DISCCART 635000. 570000. 387.
RE FINISHED
```

U.S. EPA OSW recommends that air modeling for each risk assessment include, at a minimum, an array of receptor grid nodes covering the area within 10 kilometers of the facility with the origin at the centroid of a polygon formed by the locations of the stack emission sources. This receptor grid node array should consist of a Cartesian grid with grid nodes spaced 100 meters apart extending from the centroid of the emission sources out to 3 kilometers from the centroid. For the distances from 3 kilometers out to 10 kilometers, the receptor grid node spacing can be increased to 500 meters. The single grid node array contains both grid node spacings. This same receptor grid node array is included in the REceptor pathway for all ISCST3 runs for all years of meteorological data and for all emission sources.

Terrain elevations should be specified for all receptor grid nodes. Several methods are available for assigning terrain elevations to grid nodes using digital terrain data. The 1:250,000 scale DEM digital data are available for download at the USGS Internet site:

Worldwide Web:	http://edcwww.cr.usgs.gov/pub/data/dem/250
FTP (two options):	ftp://edcwww.cr.usgs.gov/pub/data/dem/250 ftp://edcftp.cr.usgs.gov/pub/data/dem/250

This data has horizontal spacing between digital terrain values of approximately 90 meters which provides sufficient accuracy for air modeling.

In addition to the receptor grid node array evaluated for each facility out to 10 kilometers, other grid node arrays may be considered for evaluation of water bodies and their watersheds, ecosystems and special ecological habitats located beyond 10 kilometers. Grid node spacing of 500 meters between nodes is

recommended for grid node arrays positioned at distances greater than 10 kilometers from the emission source. An equally spaced grid node array facilitates subsequent computation of area averages for deposition rates.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

- Summary of all information regarding the coordinates and placement of the receptor grid node array used in air modeling
- Copies of any maps, figures, or aerial photographs used to develop the receptor grid node array
- Map presenting UTM locations of receptor grid nodes, along with other facility information.

3.7.4 MEteorological Pathway

The file containing meteorological data is specified in the MEteorological pathway. PCRAMMET creates individual files for each of 5 years, as ASCII files, to be read into ISCST3 for computing hourly concentrations and deposition rates. The modeler may specify a single year of meteorological data in each ISCST3 run, or combine the total period of meteorological data into a single meteorological file for processing by ISCST3 in a single 5-year run. When combining meteorological files, the modeler is cautioned to consider the following:

- Preprocess each year separately using PCRAMMET or MPRM into an ASCII format
- Combine the years into a single file (using a text editor or DOS COPY command)
- The first line (header) of the combined file is read by ISCST3 for comparison to the Surface and Upper Air Station ID numbers specified in the input file ME pathway
- The header for subsequent years is read by ISCST3 only if not deleted in the combined file. If subsequent year headers are included in the combined file, ISCST3 will compare the station IDs to the input file station ID. For air modeling analysis which use meteorological data from more than one surface station or upper air station (e.g., the upper air station is moved after the third year of the period and assigned a new station ID by the National Weather Service), the modeler should delete the headers for subsequent years in the combined file.

- For sites where the anemometer height is changed during the 5 year period (e.g., for the period 1984-1988, the anemometer was relocated from 20 feet to 10 meters on December 15, 1985), the modeler should run each year separately to specify the correct anemometer height in the ISCST3 input file ME pathway which corresponds to the correct height for that year of meteorological data.

Details of specifying the meteorological data file are in the ISC3 User's Guide (Section 3.5.1.1). Each year within the file must be complete with a full year of data (365 days, or 366 days for leap years). The anemometer height must be verified for the surface station from Local Climate Data Summary records, or other sources, such as the state climatologist office. U.S. EPA OSW recommends that the anemometer height ANEMHGHT for the wind speed measurements at the surface station be correctly identified before air modeling.

The following is an example input section for the MEteorological pathway, using the 1984 Baton Rouge file, with an anemometer height of 10 meters and station identification numbers:

```
ME STARTING
ME INPUTFIL 84BR.WET
ME ANEMHGHT 10.0
ME SURFDATA 13970 1984 BATON_ROUGE
ME UAIRDATA 12884 1984 BOOTHVILLE
ME FINISHED
```

3.7.5 Terrain Grid (TG) Pathway

The computation of dry plume depletion is sensitive to terrain elevation. In the absence of a terrain grid file, ISCST3 automatically assumes that the terrain slope between the stack base and the receptor grid node elevation is linear. In concept, this assumption may underestimate plume deposition. However, based on experience, the magnitude of the differences in computed concentrations and deposition rates is nominal. Since the inclusion of a terrain grid file in the TG pathway significantly increases model execution time, U.S. EPA OSW recommends that a terrain grid file is not necessary for all sites. If a terrain grid file is desired for a specific site based on highly variable terrain over short distances, the format of the TG file is described in the ISC3 User's Guide.

The location keyword of the TG pathway (`TG LOCATION`) identifies the x and y values to be added to the source and receptor grid to align with the terrain file coordinates. If the source and receptor grid nodes are in relative units such that the source is at location 0,0, the location keywords in the TG pathway would be the UTM coordinates of the source. U.S. EPA OSW requires that all emission sources and receptor grid nodes be specified in UTM coordinates (NAD27 or NAD83 format), and that the TG file, if used, be in UTM coordinates. Therefore, the location of the origin of the TG file relative to the source location will be 0,0. Also, U.S. EPA OSW recommends that the terrain elevations in the TG file be presented in meters. Following is an example of the TG pathway:

```
TG STARTING
TG INPUTFIL TERRAIN.TER
TG LOCATION 0.0 0.0
TG ELEVUNIT METERS
TG FINISHED
```

3.7.6 OUtput Pathway

ISCST3 provides numerous output file options in addition to the results in the output summary file specified in receptor tables (RECTABLE). The plot file is most useful for facilitating post-processing of the air parameter values in the model output. The plot file lists the x and y coordinates and the concentration or deposition rate values for each averaging period in a format that can be easily pulled into a post-processing program (or spreadsheet). Note that the ISCST3 generated 'plot' file is not the same format as the ISCST3 generated 'post' file. U.S. EPA OSW recommends using the plot file, not the post file.

Following is an example OUtput file specification for single-year run of 1-hour and annual average plot files:

```
OU STARTING
OU RECTABLE ALLAVE FIRST
OU PLOTFILE 1 ALL FIRST BTR841.PLT
OU PLOTFILE ANNUAL ALL BTR84A.PLT
OU FINISHED
```

For ecological risk assessments, the 1-hour average plot file is not needed. If the modeler has directed in the ISCST3 control pathway for 1-hour averages to be computed for use in a human health acute risk

assessment, then the 1-hour average plot file also should be specified (U.S. EPA 1998). The second line in the example directs ISCST3 to create a table of values for each receptor grid node for all averaging periods in the model run (annual and optionally 1-hour). The third line directs ISCST3 to create a separate plot file of the 1-hour average results, if desired by the modeler. The fourth line directs ISCST3 to create another separate plot file of the annual average results for all sources in the run for each receptor grid node.

3.8 ISCST3 MODEL EXECUTION

Model execution time should be considered for each analysis. A complete air modeling run—including air concentration, wet and dry deposition, and plume depletion—may require 10 times the run time for the same source and receptor grid nodes for air concentration only. Even if only the total deposition is specified, ISCST3 must compute air concentration and the dry and wet deposition components in order to compute the total deposition air parameter values required for the ecological risk assessment. For example, an ISCST3 particle run of one source with 800 receptor grid nodes, on 1 year of meteorological data, with the options for air concentration, wet and dry deposition, and plume depletion required about 40 hours on a personal computer with a 486 processor running at 66 megahertz (486/66). The same run can be completed in about 10 hours on a 586/120 personal computer. Five years of meteorological data and an additional 1,600 receptor grid nodes result in total run times of 120 hours for 1 year, and 600 hours for a 5-year analysis on a 486/66 personal computer. Run time on a 586/120 personal computer is estimated at about 150 hours. A significant loss of modeling effort and analysis time can be prevented by verifying input parameters and conducting test runs prior to executing the ISCST3 runs.

Long run times result mainly from two algorithms—plume depletion and terrain grid file. ISCST3 run times are increased as much as tenfold for runs applying plume depletion. U.S. EPA OSW believes that constituent mass must be conserved between suspended concentration and deposition rate by allowing for depletion of deposited mass from the plume concentration in ISCST3. The overestimate of plume concentration, and the subsequent overestimate of deposition, which results when plume depletion is not allowed, is too conservative. However, the nominal benefits of including a terrain grid file do not justify the added run times. Therefore, plume depletion should always be included, but terrain grid files are not recommended.

3.9 USE OF MODELED OUTPUT

The ISCST3 modeled output (air concentrations and deposition rates) are provided on a unit emission rate (1.0 g/s) basis from the combustion unit or emission source, and are not COPC-specific. The estimating media equations presented in Section 3.11 and Appendix B require the model output (air parameters, see Table 3-5) directly without converting the unit based output to COPC-specific output. However, there may be some instances where the risk assessor will need to convert modeled output to COPC-specific output for the risk assessment. For example, the risk assessor may want to compare modeled COPC concentrations in ambient media to concentrations actually measured in the field.

3.9.1 Unit Rate Output vs. COPC-Specific Output

The relationship between the unit emission rate and the unit air parameter values (air concentrations and deposition rates) is linear. Similarly, the relationship between the COPC-specific emission rate (Q) and the COPC-specific air parameter values (air concentrations and deposition rates) would also be linear if the COPC-specific emission rate was used in the air model. Section 3.3 discussed the use of the unit emission rate and advanced the theory that a unit emission rate should be used instead of the COPC-specific emission rate in order to preclude having to run the ISCST3 model separately for each individual COPC. The use of a unit emission rate in the air modeling is advocated because a common ratio relationship can be developed between the unit emission rate and the COPC-specific emission rate based on the fact that in the air model, both individual relationships are linear. This ratio relationship can be expressed by the following equation:

TABLE 3-5

AIR PARAMETERS FROM ISCST3 MODELED OUTPUT

Air Parameter	Description	Units
Cyv	Unitized yearly average air concentration from vapor phase	μg-s/g-m^3
Cyp	Unitized yearly average air concentration from particle phase	μg-s/g-m^3
Dywv	Unitized yearly average wet deposition from vapor phase	s/m^2-yr
Dydp	Unitized yearly average dry deposition from particle phase	s/m^2-yr
Dywp	Unitized yearly average wet deposition f rom particle phase	s/m^2-yr
Cywv	Unitized yearly (water body or watershed) average air concentration from vapor phase	μg-s/g-m^3
Dywwv	Unitized yearly (water body or watershed) average wet deposition from vapor phase	s/m^2-yr
Dytwp	Unitized yearly (water body or watershed) average total (wet and dry) deposition from particle phase	s/m^2-yr

$$\frac{\text{COPC-Specific Air Concentration}}{\text{COPC-Specific Emission Rate}} = \frac{\text{Modeled Output Air Concentration}}{\text{Unit Emission Rate}} \qquad \text{Equation 3-2}$$

Use of this equation requires that three of the variables be known. The modeled output air concentration (or deposition rate) is provided by the air model, the unit emission is 1.0 g/s, and the COPC-specific emission rate; which is obtained directly from stack or source test data.

3.9.1.1 Determination of the COPC-Specific Emission Rate (*Q*)

The COPC-specific emission rate can usually be determined with information obtained directly from the trial burn report. The COPC-specific emission rate from the stack is a function of the stack gas flow rate and the stack gas concentration of each COPC; which can be calculated from the following equation:

$$Q = SGF \cdot \frac{SGC \cdot CFO_2}{1 \times 10^6} \qquad \text{Equation 3-4}$$

where

Q	=	COPC-specific emission rate (g/s)
SGF	=	Stack gas flow rate at dry standard conditions (dscm/s)
SGC	=	COPC stack gas concentration at 7 percent O_2 as measured in the trial burn (µg/dscm)
CFO_2	=	Correction factor for conversion to actual stack gas concentration O_2 (unitless)
1 x 10^6	=	Unit conversion factor (µg/g)

Guidance for determining COPC-specific emission rates for fugitive emission sources can be found in Chapter 2. Also, it is sometimes necessary to derive the COPC-specific emission rate from surrogate data, such as for a new facility that has not yet been constructed and trial burned (see Chapter 2).

3.9.1.2 Converting Unit Output to COPC-Specific Output

Once the three of the four variables in Equation 3-1 are known, the COPC-specific air concentrations and deposition rates can be obtained directly by multiplication, as follows:

$$\text{COPC-Specific Air Concentration} = \frac{\text{Modeled Output Air Concentration} \cdot \text{COPC-Specific Emission Rate}}{\text{Unit Emission Rate}} \qquad \text{Equation 3-3}$$

For example, if COPC A is emitted at a rate of 0.25 g/s, and the ISCST3 modeled concentration at a specific receptor grid node is 0.2 μg/m^3 per the 1.0 g/s unit emission rate, the concentration of COPC A at that receptor grid node is 0.05 μg/m^3 (0.25 multiplied by 0.2). Deposition is calculated similarly, proportional to the emission rate of each COPC. Readers are reminded once again that this process of

converting modeled unitized output into COPC-specific output is taken directly into account in the estimating media concentration equations in Section 3.11 and Appendix B.

3.9.2 Output from the ISCST3 Model

The ISCST3 output is structured and the risk assessor must understand how to read the output in order to ensure accurate use of modeled output in the risk assessment. The output from each ISCST3 model run is written to two separate file formats. The 'output file' is specified by name at run time in the execution command. Typical command line nomenclature is:

```
ISCST3 inputfile.INP outputfile.OUT
```

where

`ISCST3`:	specifies execution of the ISCST3 model
`inputfile.INP`:	is the input file name selected by the modeler
`outputfile.OUT`:	is the output file name selected by the modeler, typically the same as the input file name

For example, the following ISCST3 input line would run the input file (PART84.INP) created by the modeler for particulate emissions using 1984 meteorological data. The output file (PART84.OUT) from the run will automatically be written by ISCST3 during model execution.

```
ISCST3 PART84.INP PART84.OUT
```

The output 'plot file' is specified by the modeler in the ISCST3 input file OUtput pathway and created by ISCST3 during the run (see Section 3.7.6). Figure 3-3 is an example of the first few lines in the particle phase plot file with single-year annual average concentration, total deposition, dry deposition and wet deposition values for each receptor grid node. The total deposition is the sum of the dry and wet components of deposition. The single-year values at each receptor grid node being evaluated must be averaged to a 5-year value. The 5-year averaged values at the receptor grid nodes selected for evaluation in the risk assessment (see Section 3.9.3), are used in the estimating media concentration equations. This file is usually imported into a post-processing program (or spreadsheet) before entry into the risk assessment computations.

Similar plot files are produced for the particle-bound and vapor phase runs. The output for the vapor phase runs will be average concentration and wet deposition. The output for the particle and particle-bound phase runs will be average concentration, dry deposition, wet deposition and total deposition. Again, the 1-year values at each receptor grid node must be averaged to a 5-year value at each node unless a single five-year ISCST3 run using a combined meteorological file is used. If the 5-year combined file is used, the results from the ISCST3 plot file may be used directly in the risk assessment without averaging over the five years.

All values are defined as used in the estimating media concentration equations (see Section 3.11).

3.9.3 Use of Model Output in Estimating Media Equations

Section 3.4 discussed how consideration of partitioning of the COPCs effects the development of ISCST3 modeling runs. The selection of which air modeled air parameter values (air concentrations and deposition rates) to use in the estimating media concentration equations is based on this same partitioning theory.

3.9.3.1 Vapor Phase COPCs

ISCST3 output generated from vapor phase air modeling runs are vapor phase air concentrations (unitized *Cyv* and unitized *Cywv*) and wet vapor depositions (unitized *Dywv* and unitized *Dywwv*) for organic COPCs at receptor grid nodes based on the unit emission rate. These values are used in the estimating media concentration equations for all COPC organics except the polycyclic aromatic hydrocarbons dibenzo(a,h)anthracene and indeno(1,2,3-cd)pyrene, which have vapor phase fractions, Fv, less than five percent. The air concentration (unitized *Cyv*) and wet vapor deposition (unitized *Dywv*) from the vapor phase run is also used in the estimating media concentration equations for mercury. Values for these COPCs are selected from the vapor phase run because the mass of the COPC emitted by the combustion unit is assumed to have either all or a portion of its mass in the vapor phase (see Appendix A-2).

3.9.3.2 Particle Phase COPCs

ISCST3 output generated from particle phase air modeling runs are air concentration (unitized *Cyp*), dry deposition (unitized *Dydp*), wet deposition (unitized *Dywp*), and combined deposition (unitized *Dytwp*) for inorganics and relatively non-volatile organic COPCs at receptor grid nodes based on the unit emission rate. These values are used in the estimating media concentration equations for all COPC inorganics (except mercury, see Chapter 2 and Appendix A-2) and polycyclic aromatic hydrocarbons with fraction of vapor phase, Fv , less than 0.05 (e.g., dibenzo(a,h)anthracene and indeno(1,2,3-cd)pyrene). Values for inorganic and relatively non-volative COPCs are selected from the particle phase run because the mass of the COPC emitted by the combustion unit is assumed to have all of its mass in the particulate phase (see Appendix A-2), apportioned across the particle size distribution based on mass weighting.

3.9.3.3 Particle-Bound COPCs

ISCST3 output generated from particle-bound air modeling runs are air concentration (unitized *Cyp*), dry deposition (unitized *Dydp*), wet deposition (unitized *Dywp*), and combined deposition (unitized *Dytwp*) for organic COPCs and mercury (see Chapter 2 and Appendix A-2) at receptor grid nodes based on the unit emission rate. These values are used in the estimating media concentration equations for all COPC organics and mercury to account for a portion of the vapor condensed onto the surface of particulates. Values for these COPCs are selected from the particle-bound run because the mass of the COPC emitted by the combustion unit is assumed to have a portion of its mass condensed on particulates (see Appendix A-2), apportioned across the particle size distribution based on surface area weighting.

3.10 MODELING OF FUGITIVE EMISSIONS

Fugitive source emissions, as defined in Chapter 2, should be modeled using the procedures presented throughout this chapter for stack source emissions. However, the fugitive emissions should be represented in the ISCST3 input file SOurce pathway as either “area” or “volume” source types. Fugitive emissions of volatile organics are modeled only in the vapor phase. Fugitive emissions of ash are modeled only in the particle and particle-bound phases, not vapor phase.

As discussed in Chapter 2, fugitive emissions of volatile organic vapors are associated with combustion units that include storage vessels, pipes, valves, seals and flanges. The horizontal area of the fugitive source (which can be obtained from the facility plot plan) is entered into the ISCST3 input file following the instructions presented in the ISC3 User's Guide, Volume I (U.S. EPA 1995c). The height of the fugitive source is defined as the top of the vertical extent of the equipment. If the vertical extent of the fugitive source is not known, a default height of ground level (release height of zero) may be input, providing a conservative estimate of potential impacts. The ISCST3 model run time is faster for volume source types than for area source types, and should be considered for most applications. The methods in the ISCST3 User's Guide should be followed in defining the input parameters to represent the fugitive source.

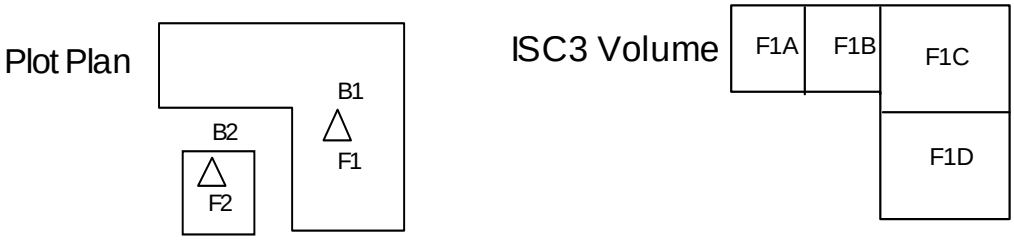
FIGURE 3-3

EXAMPLE PLOT FILE

```
*ISCST3 (96113):  Example Particle Phase Run, Single Year 1990
*MODELING OPTIONS USED:
* CONC   DEPOS  DDEP   WDEP   RURAL  ELEV          DFAULT                                        DRYDPL WETDPL

*        PLOT FILE OF ANNUAL VALUES FOR SOURCE GROUP: ALL
*        FOR A TOTAL OF    21 RECEPTORS.
*        FORMAT: (6(1X,F13.5),1X,F8.2,2X,A6,2X,A8,2X,I8,2X,A8)
*     X            Y        AVERAGE CONC  TOTAL DEPO    DRY DEPO      WET DEPO   ZELEV      AVE   GRP   NUM HRS   NET
ID
*_____________ _____________  ___________   _________   ___________  _________  _______  _______  _____ ________
_________
691600.00000 3342050.00000     0.29900     0.28658       0.20024      0.08634     4.00     ANNUAL  ALL    8760     NA
691700.00000 3342050.00000     0.30203     0.35416       0.23884      0.11532     5.00     ANNUAL  ALL    8760     NA

691800.00000 3342050.00000     0.25174     0.42461       0.25976      0.16485     5.00     ANNUAL  ALL    8760     NA

691900.00000 3342050.00000     0.13256     0.50524       0.23852      0.26672     5.00     ANNUAL  ALL    8760     NA

692000.00000 3342050.00000     0.00322     0.61790       0.05850      0.55940     5.00     ANNUAL  ALL    8760     NA

692100.00000 3342050.00000     0.00000     6.32022       0.00000      6.32022     6.00     ANNUAL  ALL    8760     NA

692200.00000 3342050.00000     0.00319     0.32218       0.06577      0.25641     6.00     ANNUAL  ALL    8760     NA

692300.00000 3342050.00000     0.13768     0.39938       0.21734      0.18204     6.00     ANNUAL  ALL    8760     NA

692400.00000 3342050.00000     0.23546     0.33855       0.20975      0.12880     6.00     ANNUAL  ALL    8760     NA

692500.00000 3342050.00000     0.25673     0.27475       0.17903      0.09572     6.00     ANNUAL  ALL    8760     NA

692600.00000 3342050.00000     0.24706     0.22195       0.14812      0.07384     6.00     ANNUAL  ALL    8760     NA

691600.00000 3342150.00000     0.37348     0.40644       0.25958      0.14685     5.00     ANNUAL  ALL    8760     NA

691700.00000 3342150.00000     0.37166     0.51388       0.31119      0.20269     5.00     ANNUAL  ALL    8760     NA
```

691800.00000	3342150.00000	0.34332	0.68794	0.39582	0.29212	5.00	ANNUAL	ALL	8760	NA
691900.00000	3342150.00000	0.22930	0.98039	0.54883	0.43156	5.00	ANNUAL	ALL	8760	NA
692000.00000	3342150.00000	0.03473	0.90823	0.37421	0.53402	6.00	ANNUAL	ALL	8760	NA
692100.00000	3342150.00000	0.00098	0.62882	0.15736	0.47146	6.00	ANNUAL	ALL	8760	NA
692200.00000	3342150.00000	0.02605	0.48160	0.15582	0.32578	7.00	ANNUAL	ALL	8760	NA
692300.00000	3342150.00000	0.17300	0.49313	0.22998	0.26315	7.00	ANNUAL	ALL	8760	NA
692400.00000	3342150.00000	0.24520	0.29443	0.19715	0.09729	7.00	ANNUAL	ALL	8760	NA
692500.00000	3342150.00000	0.25561	0.23482	0.16744	0.06738	7.00	ANNUAL	ALL	8760	NA

The following example is for organic fugitive emissions modeled as a volume source type. For a facility which may have two stack emission sources (B1, B2) and two fugitive emission sources (areas F1, F2); a total of four runs for each year (or 5-year combined file) of meteorological data is required. One run is required for each of the two stacks as point sources. One run is required for each of the two fugitive areas as volume sources (Note: modeler may alternatively model as an area source). Since the emissions are fugitive volatile organics, only the vapor phase is modeled. The vertical extent of the pipes, valves, tanks and flanges associated with each fugitive emission area is 15 feet (about 5 meters) above plant elevation. To define the sources for input to ISCST3, the release height is specified as 2.5 meters (½ of vertical extent of fugitive emissions). The initial vertical dimension is specified as 1.16 meters (vertical extent of 5 meters divided by 4.3 as described in the ISC3 User's Guide).



The initial horizontal dimension is the side length of the square fugitive area (footprint) divided by 4.3. If fugitive area F2 has a measured side of 30 meters, the initial horizontal dimension is 6.98 (30 meters divided by 4.3). For fugitive area F1, the area on the plot plan must be subdivided (ISC3 Volume) to create square areas for input to ISCST3. The four areas depicted represent subdivision into square areas. The resulting four square areas are input into a single ISCST3 run for Fugitive source F1 as four separate volume sources (F1A, F1B, F1C, F1D). The initial horizontal dimension for each volume source is the side of the square divided by 4.3. It is very important to allocate proportionately the unit emission rate (1.0 gram per second) among the subdivided areas. For example, if the areas of the subdivided squares in the ISC3 Volume figure results in F1A equal to F1B each with 1/8th the total area, the proportion of the unit emissions allocated to each of these volume sources is 0.125 grams per second. The remaining two areas are each 3/8ths of the total area of fugitive F1, so that 0.375 grams per second is specified for the emission rate from each source. The total emissions for the four volume sources sum to the unit emission rate for the F1 fugitive source (0.125 + 0.125 + 0.375 + 0.375 = 1.0 g/s). By specifying all sources to be included in the model results from ISCST3 (SO SRCGROUP ALL), the ISCST3 model will appropriately

combine all four volume source subdivisions of fugitive source F1 into combined impact results for fugitive source F1. The resulting air parameter values in the plot files may be used directly in the risk assessment equations, the same as if a stack emission were modeled as a single point source. The initial vertical dimension is defined the same as F2, using the vertical extent of 5 meters divided by 4.3 and a release height of 2.5 meters (½ vertical extent). For volume sources, the location is specified by the x and y coordinates of the center of each square area.

The COntrol parameters should follow the recommendations for setting up a vapor phase computation.

```
CO CONC WDEP
```

Fugitive emissions of ash particles are from the storage piles associated with combustion units. The horizontal area of the storage pile is entered into the ISCST3 input file following the ISCST3 User's Guide, Volume I (U.S. EPA 1995c). The height of emissions is input as the top of the pile. If the vertical extent is not known, the height may be input as ground level (or zero height). Fugitive ash will typically be modeled as area source type. However, volume source type may be considered by the appropriate regulatory agency prior to air modeling. The methods in the ISCST3 User's Guide should be followed in defining the input parameters to represent the ash release as an area source.

The COntrol parameters should follow the recommendations for setting up a particulate phase computation.

```
CO CONC DDEP WDEP DEPOS
```

The emissions characterization and source type must be documented.

3.11 ESTIMATION OF COPC CONCENTRATIONS IN MEDIA

As discussed in Section 3.9 (see also Table 3-5), the ISCST3 modeled output of unitized air parameters (air concentrations and deposition rates) are provided on a unit emission (1.0 g/s) basis from the combustion unit, and are not COPC-specific. The estimating media concentration equations, presented in this section, accept these unitized output values directly to calculate COPC-specific media concentrations

for use in characterizing ecological risk. Selection of the appropriate ISCST3 modeled output for use in the equations is discussed in Section 3.9.

This section presents the estimating media concentration equations used for calculating, from the appropriate ISCST3 unitized model output and COPC-specific emission rates, COPC-specific media concentrations in soil, surface water, and sediment. Determining COPC media concentrations is relevant to estimating risks to potentially impacted ecosystems through exposure of ecological receptors to COPCs in air (plant only), soil, surface water, and sediment. This section also includes equations for calculating COPC-specific concentrations in terrestrial plants resulting from foliar and root uptake.

Section 3.11.1 describes the equations for calculating COPC-specific concentration in soils. Section 3.11.2 describes the equations for calculating COPC-specific concentrations in surface water and sediment. Section 3.11.3 describes the equations for calculating COPC-specific plant concentrations from foliar and root uptake. In addition, Appendix B also provides in more detail the media concentration equations and default input variables recommended by U.S. EPA OSW.

3.11.1 CALCULATION OF COPC CONCENTRATIONS IN SOIL

As depicted in Figure 3-4, COPC concentrations in soil are calculated by summing the particle and vapor phase deposition of COPCs to the soil. Wet and dry deposition of particles and vapors are considered, with dry deposition of vapors calculated from the vapor air concentration and the dry deposition velocity. Soil concentrations may require many years to reach steady state. As a result, the equations used to calculate the soil concentration over the period of deposition were derived by integrating the instantaneous soil concentration equation over the period of deposition. U.S. EPA OSW recommends that the highest 1-year annual average COPC concentration in soil be used as the soil concentration for estimating ecological risk, which would typically occur at the end of the time period of combustion (see Section 3.11.1).

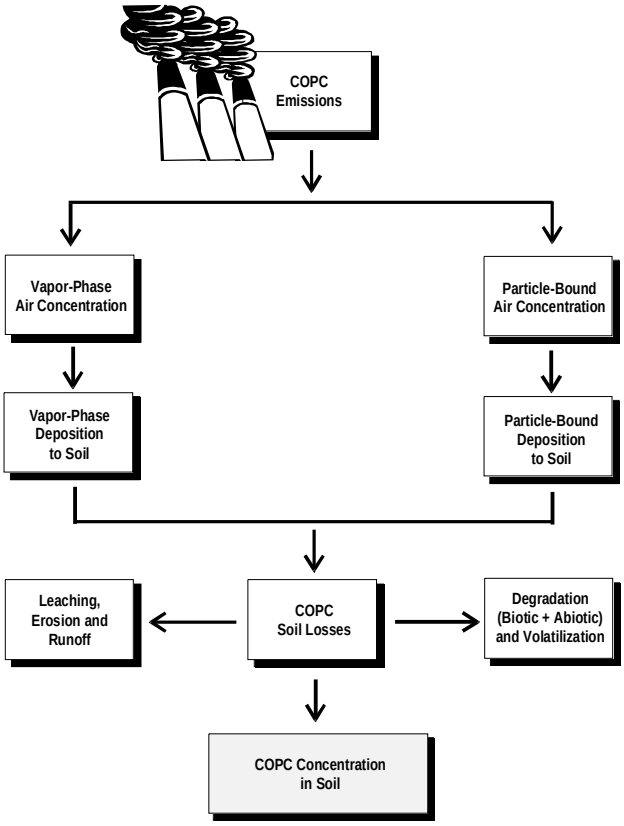


Figure 3-4 - COPC Concentration in Soil

Following deposition, the calculation of soil concentration also considers losses of COPCs by several mechanisms, including leaching, erosion, runoff, degradation (biotic and abiotic), and volatilization. All of these loss mechanisms may lower the soil concentration if included in the soil concentration calculation (see Section 3.11.1.2). Soil conditions—such as pH, structure, organic matter content, and moisture content—can also affect the distribution and mobility of COPCs in soil. Loss of COPCs from the soil is modeled using a combination of default and site-specific values to account for the physical and chemical characteristics of the soil.

COPCs may also be physically incorporated into the upper layers of soil through tilling. The concentration in the top 20 centimeters of soil should be computed for estimating a COPC concentration in soils that are

physically disturbed or tilled. The COPC concentration in the top 1 centimeter of soil should be computed for estimating a COPC concentration in soils that are not tilled (see Section 3.11.1.4).

3.11.1.1 Calculating Highest Annual Average COPC Concentration in Soil

U.S. EPA OSW recommends the following equation for calculating the highest average annual COPC soil concentration.

Recommended Equations for Calculating:
Highest Annual Average COPC Concentration in Soil (*Cs*)

$$Cs = \frac{Ds \cdot [1 - \exp(-ks \cdot tD)]}{ks}$$ Equation 3-7

where

Cs	=	COPC concentration in soil (mg COPC/kg soil)
Ds	=	Deposition term (mg/kg-yr)
ks	=	COPC soil loss constant due to all processes (yr^{-1})
tD	=	Total time period over which deposition occurs (time period of combustion) (yr)

This equation calculates the highest annual average soil concentration, which is typically expected to occur at the end of the time period of deposition (U.S. EPA 1994l; 1998c). Derivation of the equation is presented in U.S. EPA (1998c). Appendix B, Table B-1-1 also describes the equation, definitions of its terms, and default values for the variables.

3.11.1.2 Calculating the COPC Soil Loss Constant (*ks*)

COPCs may be lost from the soil by several processes that may or may not occur simultaneously. In Equation 3-8, the soil loss constant, *ks*, expresses the rate at which a COPC is lost from soil (U.S. EPA 1993h; 1998c). The constant *ks* is determined by using the soil's physical, chemical, and biological characteristics to consider the losses resulting from:

(1) biotic and abiotic degradation,

(2) erosion,

(3) surface runoff,

(4) leaching, and

(5) volatilization.

Consistent with earlier U.S. EPA guidance (U.S. EPA 1993h; 1994l; 1998c), U.S. EPA OSW recommends using Equation 3-8 to compute the soil loss constant.

Recommended Equation for Calculating:
COPC Soil Loss Constant (*ks*)

$$ks = ksg + kse + ksr + ksl + ksv \qquad \text{Equation 3-8}$$

where

ks	=	COPC soil loss constant due to all processes (yr^{-1})
ksg	=	COPC loss constant due to degradation (yr^{-1})
kse	=	COPC loss constant due to erosion (yr^{-1})
ksr	=	COPC loss constant due to runoff (yr^{-1})
ksl	=	COPC loss constant due to leaching (yr^{-1})
ksv	=	COPC loss constant due to volatilization (yr^{-1})

The use of Equation 3-8 assumes that COPC loss can be defined by using first-order reaction kinetics. First-order reaction rates depend on the concentration of one reactant (Bohn, McNeal, and O'Connor 1985). The loss of a COPC by a first-order process depends only on the concentration of the COPC in the soil, and a constant fraction of the COPC is removed from the soil over time. Those processes that apparently exhibit first-order reaction kinetics without implying a mechanistic dependence on a first-order loss rate are termed "apparent first-order" loss rates (Sparks 1989). The assumption that COPC loss follows first-order reaction kinetics may be an oversimplification because—at various concentrations or under various environmental conditions—the loss rates from soil systems will resemble different kinetic expressions. However, at low concentrations, a first-order loss constant may be adequate to describe the loss of the COPC from soil (U.S. EPA 1990a).

COPC loss in soil can also follow zero or second-order reaction kinetics. Zero-order reaction kinetics are independent of reactant concentrations (Bohn, McNeal, and O'Connor 1985). Zero-order loss rates describe processes in which the reactants are present at very high concentrations. Under zero-order kinetics, a constant amount of a COPC is lost from the soil over time, independent of its concentration. Processes that follow second-order reaction kinetics depend on the concentrations of two reactants or the concentration of one reactant squared (Bohn, McNeal, and O'Connor 1985). The loss constant of a COPC following a second-order process can be contingent on its own concentration, or on both its concentration and the concentration of another reactant, such as an enzyme or catalyst.

Because COPC loss from soil depends on many complex factors, it may be difficult to model the overall rate of loss. In addition, because the physical phenomena that cause COPC loss can occur simultaneously, the use of Equation 3-8 may also overestimate loss rates for each process (Valentine 1986). When possible, the common occurrence of all loss processes should be taken into account.

The following subsections discuss issues associated with the calculation of the *ksl*, *kse*, *ksr*, *ksg*, and *ksv* variables. Appendix B, Tables B-1-2 through B-1-6 present the equations for computing the overall and individual soil loss constant, except for loss due to degradation, which is discussed below.

COPC Loss Constant Due to Biotic and Abiotic Degradation *(ksg)*

Soil losses resulting from biotic and abiotic degradation (*ksg*) are determined empirically from field studies and should be addressed in the literature (U.S. EPA 1990a). Lyman et al. (1982) states that degradation rates can be assumed to follow first order kinetics in a homogenous media. Therefore, the half-life of a compound can be related to the degradation rate constant. Ideally, *ksg* is the sum of all biotic and abiotic rate constants in the soil media. Therefore, if the half-life of a compound (for all of the mechanisms of transformation) is known, the degradation rate can be calculated. However, literature sources do not provide sufficient data for all such mechanisms, especially for soil. Therefore, Appendix A-2 presents U.S. EPA OSW recommended values for this COPC specific variable.

Recommended Values for:
COPC Loss Constant Due to Biotic and Abiotic Degradation (*ksg*)

See Appendix A-2

The rate of biological degradation in soils depends on the concentration and activity of the microbial populations in the soil, the soil conditions, and the COPC concentration (Jury and Valentine 1986). First-order loss rates often fail to account for the high variability of these variables in a single soil system. However, the use of simple rate expressions may be appropriate at low chemical concentrations (e.g., nanogram per kilogram soil) at which a first-order dependence on chemical concentration may be reasonable. The rate of biological degradation is COPC-specific, depending on the complexity of the COPC and the usefulness of the COPC to the microorganisms. Some substrates, rather than being used by the organisms as a nutrient or energy source, are simply degraded with other similar COPCs, which can be further utilized. Environmental and COPC-specific factors that may limit the biodegradation of COPCs in the soil environment (Valentine and Schnoor 1986) include:

(1) availability of the COPC,

(2) nutrient limitations,

(3) toxicity of the COPC, and

(4) inactivation or nonexistence of enzymes capable of degrading the COPC.

Chemical degradation of organic compounds can be a significant mechanism for removal of COPCs in soil (U.S. EPA 1990a). Hydrolysis and oxidation-reduction reactions are the primary chemical transformation processes occurring in the upper layers of soils (Valentine 1986). General rate expressions describing the transformation of some COPCs by all non-biological processes are available, and these expressions are helpful when division into component reactions is not possible.

Hydrolysis in aqueous systems is characterized by three processes: acid-catalyzed, base-catalyzed, and neutral reactions. The overall rate of hydrolysis is the sum of the first-order rates of these processes (Valentine 1986). In soil systems, sorption of the COPC can increase, decrease, or not affect the rate of hydrolysis, as numerous studies cited in Valentine (1986) have shown. The total rate of hydrolysis in soil can be predicted by adding the rates in the soil and water phases, which are assumed to be first-order

reactions at a fixed pH (Valentine 1986). Methods for estimating these hydrolysis constants are described by Lyman et al. (1982).

Organic and inorganic compounds also undergo oxidation-reduction (redox) reactions in the soil (Valentine 1986). Organic redox reactions involve the exchange of oxygen and hydrogen atoms by the reacting molecules. Inorganic redox reactions may involve the exchange of atoms or electrons by the reactants. In soil systems where the identities of oxidant and reductant species are not specified, a first-order rate constant can be obtained for describing loss by redox reactions (Valentine 1986). Redox reactions involving metals may promote losses from surface soils by making metals more mobile (e.g., leaching to subsurface soils).

COPC Loss Constant Due to Soil Erosion (*kse*)

U.S. EPA (1993h) recommended the use of Equation 3-8A to calculate the constant for soil loss resulting from erosion (*kse*).

$$kse = \frac{0.1 \cdot X_e \cdot SD \cdot ER}{BD \cdot Z_s} \cdot \frac{Kd_s \cdot BD}{\theta_{sw} + (Kd_s \cdot BD)} \qquad \text{Equation 3-8A}$$

where:

kse	=	COPC soil loss constant due to soil erosion
0.1	=	Units conversion factor (1,000 g-kg/10,000 cm^2-m^2)
X_e	=	Unit soil loss (kg/m^2-yr)
SD	=	Sediment delivery ratio (unitless)
ER	=	Soil enrichment ratio (unitless)
Kd_s	=	Soil-water partition coefficient (mL/g)
BD	=	Soil bulk density (g/cm^3 soil)
Z_s	=	Soil mixing zone depth (cm)
θ_{sw}	=	Soil volumetric water content (mL/cm^3 soil)

Unit soil loss (X_e) is calculated by using the Universal Soil Loss Equation (USLE), as described in Section 3.11.2. Variables associated with Equation 3-8A are further discussed in Appendix B, Table B-1-3.

U.S. EPA guidance (1994b and 1994l) have stated that all *kse* values are equal to zero. U.S. EPA (1994l) stated that *kse* is equal to zero because of contaminated soil eroding onto and off of the site.

Consistent with earlier U.S. EPA guidance (1994b and 1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends that the constant for the loss of soil resulting from erosion (*kse)* should be set equal to zero.

Recommended Value for: COPC Loss Constant Due to Erosion (*kse*)
0

For additional information on addressing *kse*, U.S. EPA OSW recommends consulting the methodologies described in U.S. EPA document, *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (U.S. EPA In Press). The use of *kse* values is also further described in Appendix B, Table B-1-3.

COPC Loss Constant Due to Runoff (*ksr*)

Consistent with earlier U.S. EPA guidance (1993h; 1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends that Equation 3-8B be used to calculate the constant for the loss of soil resulting from surface runoff (*ksr*). The use of this equation is further described in Appendix B, Table B-1-4.

Recommended Equation for Calculating: COPC Loss Constant Due to Runoff (*ksr*)

$$ksr = \frac{RO}{\theta_{sw} \cdot Z_s} \cdot \left(\frac{1}{1 + \left(Kd_s \cdot BD / \theta_{sw} \right)} \right) \qquad \text{Equation 3-8B}$$

where

ksr	=	COPC loss constant due to runoff (yr^{-1})
RO	=	Average annual surface runoff from pervious areas (cm/yr)
θ_{sw}	=	Soil volumetric water content (mL/cm^3 soil)

Z_s	=	Soil mixing zone depth (cm)
Kd_s	=	Soil-water partition coefficient (mL/g)
BD	=	Soil bulk density (g/cm^3 soil)

COPC Loss Constant Due to Leaching (*ksl*)

Consistent with earlier U.S. EPA guidance (1993h and 1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends that Equation 3-8C be used to calculate the COPC loss constant due to leaching (*ksl)*. The use of this equation is further described in Appendix B, Table B-1-5.

Recommended Equation for Calculating:
COPC Loss Constant Due to Leaching (*ksl*)

$$ksl = \frac{P + I - RO - E_v}{\theta_{sw} \cdot Z_s \cdot [1.0 + (BD \cdot Kd_s / \theta_{sw})]}$$ Equation 3-8C

where

ksl	=	COPC loss constant due to leaching (yr^{-1})
P	=	Average annual precipitation (cm/yr)
I	=	Average annual irrigation (cm/yr)
RO	=	Average annual surface runoff from pervious areas (cm/yr)
E_v	=	Average annual evapotranspiration (cm/yr)
θ_{sw}	=	Soil volumetric water content (mL/cm^3 soil)
Z_s	=	Soil mixing zone depth (cm)
Kd_s	=	Soil-water partition coefficient (mL/g)
BD	=	Soil bulk density (g/cm^3 soil)

Appendix B, Table B-1-5 further describes the variables associated with Equation 3-8C. The average annual volume of water ($P + I - RO - E_v$) available to generate leachate is the mass balance of all water inputs and outputs from the area under consideration.

COPC Loss Constant Due to Volatilization (*ksv*)

Semi-volatile and volatile COPCs emitted in high concentrations may become adsorbed to soil particles and exhibit volatilization losses from soil. The loss of a COPC from the soil by volatilization depends on the rate of movement of the COPC to the soil surface, the chemical vapor concentration at the soil surface, and the rate at which vapor is carried away by the atmosphere (Jury 1986).

Consistent with U.S. EPA (In Press), U.S. EPA OSW recommends that Equation 3-8D be used to calculate the constant for the loss of soil resulting from volatilization (*ksv)*. The soil loss constant due to volatilization (*ksv*) is based on gas equilibrium coefficients and gas phase mass transfer. The first order decay constant, *ksv*, is obtained by adapting the Hwang and Falco equation for soil vapor phase diffusion (Hwang and Falco 1986). The use of this equation is further described in Appendix B, Table B-1-6.

Recommended Equation for Calculating:
COPC Loss Constant Due to Volatilization (*ksv*)

$$ksv = \left(\frac{3.1536 \times 10^{7} \cdot H}{Z_s \cdot Kd_s \cdot R \cdot T_a \cdot BD} \right) \cdot \left(\frac{D_a}{Z_s} \right) \cdot \left[1 - \left(\frac{BD}{\rho_s} \right) - \Theta_{sw} \right] \qquad \text{Equation 3-8D}$$

where

ksv	=	COPC loss constant due to volatization (yr^{-1})
3.1536×10^7	=	Units conversion factor (s/yr)
H	=	Henry's Law constant (atm-m^3/mol)
Z_s	=	Soil mixing zone depth (cm)
Kd_s	=	Soil-water partition coefficient (mL/g)
R	=	Universal gas constant (atm-m^3/mol-K)
T_a	=	Ambient air temperature (K) = 298.1 K
BD	=	Soil bulk density (g/cm^3 soil)
D_a	=	Diffusivity of COPC in air (cm^2/s)
θ_{sw}	=	Soil volumetric water content (mL/cm^3 soil)
ρ_s	=	Solids particle density (g/cm^3)

Appendix B, Table B-1-5 further describes the variables associated with Equation 3-8C. In cases where high concentrations of volatile organic compounds are expected to be present in the soil, U.S. EPA OSW

recommends consulting the methodologies described in U.S. EPA document, *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (U.S. EPA In Press). The use of *ksv* values is also further described in Appendix B, Table B-1-6.

3.11.1.3 Deposition Term (*Ds*)

U.S. EPA OSW recommends that Equation 3-9 be used to calculate the deposition term *(Ds)*. This equation is further described in Appendix B, Table B-1-1. The use of Equation 3-11 to calculate the deposition term is consistent with earlier U.S. EPA guidance (1994l) and U.S. EPA (1998c), which both incorporate a deposition term (*Ds*) into Equation 3-7 for the calculation of the COPC concentration in soil (*Cs*) (see also Section 3.11.1.1).

Recommended Equation for Calculating:
Deposition Term (*Ds*)

$$Ds = \left[\frac{100 \cdot Q}{Z_s \cdot BD}\right] \cdot [F_v(0.31536 \cdot Vdv \cdot Cyv + Dywv) + (Dywp + Dydp) \cdot (1 - F_v)] \quad \text{Equation 3-9}$$

where

Ds	=	Deposition term (mg COPC/kg soil-yr)
100	=	Units conversion factor (m^2-mg/cm^2-kg)
Q	=	COPC-specific emission rate (g/s)
Z_s	=	Soil mixing zone depth (cm)
BD	=	Soil bulk density (g/cm^3 soil)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
0.31536	=	Units conversion factor (m-g-s/cm-μg-yr)
Vdv	=	Dry deposition velocity (cm/s)
Cyv	=	Unitized yearly average air concentration from vapor phase (μg-s/g-m^3)
Dywv	=	Unitized yearly average wet deposition from vapor phase (s/m^2 year)
Dydp	=	Unitized yearly average dry deposition from particle phase (s/m^2 year)
Dywp	=	Unitized yearly average wet deposition from particle phase (s/m^2 year)

Section 3.9 further describes the ISCST3 unitized air parameters (*Cyv*, *Dywv*, *Dydp*, and *Dywp*) obtained as output from the air dispersion modeling. Appendix B describes the determination of other variables

associated with Equation 3-9. The proper use of this equation is also further described in Appendix B, Table B-1-1.

3.11.1.4 Site-Specific Parameters for Calculating Soil Concentration

As discussed in the previous sections, calculating the COPC concentration in soil (*Cs*) requires some site-specific parameter values, which must be calculated or derived from available literature or site-specific data. These site-specific parameters include the following:

- Soil mixing zone depth (Z_s)
- Soil bulk density (*BD*)
- Available water ($P + I - RO - E_v$)
- Soil volumetric water content (θ_{sw})

Determination of values for these parameters is further described in the following subsections, and in Appendix B.

Soil Mixing Zone Depth (Z_s)

When exposures to COPCs in soils are modeled, the depth of contamination is important in calculating the appropriate soil concentration. Due to leaching and physical disturbance (e.g., tilling) COPCs may migrate deeper in the soil in for some areas. Therefore, the value for the depth of soil contamination, or soil mixing zone depth (Z_s), used in modeling ecological risk should be considered specific to tilled (e.g., large plowed field) or untilled soil areas.

In general, previous U.S. EPA combustion risk assessment guidance (1990a) has estimated that if the area under consideration is tilled or mechanically disturbed, the soil mixing zone depth is about 10 to 20 centimeters depending on local conditions and the equipment used. If soil is not moved, COPCs are assumed to be retained in the shallower, upper soil layer. In this case, earlier U.S. EPA guidances (U.S. EPA 1990a; U.S. EPA 1993h) have typically recommended a value of 1 centimeter.

Consistent with earlier U.S. EPA guidance (1990a) and U.S. EPA (1998c), U.S. EPA OSW recommends the following values for the soil mixing zone depth (Z_s).

Recommended Values for: Soil Mixing Zone Depth (Z_s)
1 cm - untilled 20 cm - tilled

Soil Bulk Density (*BD*)

BD is the ratio of the mass of soil to its total volume. This variable is affected by the soil structure, type, and moisture content (Hillel 1980). Consistent with U.S. EPA (1990a; 1994b) and information presented in Hoffman and Baes (1979), U.S. EPA OSW recommends the following value for the soil dry bulk density (*BD*).

Recommended Value for: Soil Dry Bulk Density (*BD*)
1.50 g/cm^3 soil

For determination of actual field values specific to a specified location at a site, U.S. EPA (1994l) recommended that wet soil bulk density be determined by weighing a thin-walled, tube soil sample (e.g., a Shelby tube) of known volume and subtracting the tube weight (ASTM Method D2937). Moisture content can then be calculated (ASTM Method 2216) to convert wet soil bulk density to dry soil bulk density.

Available Water ($P + I - RO - E_v$)

The average annual volume of water available ($P + I - RO - E_v$) for generating leachate is the mass balance of all water inputs and outputs from the area under consideration. A wide range of values for these variables may apply in the various U.S. EPA regions.

The average annual precipitation (*P*), irrigation (*I*), runoff (*RO*), and evapotranspiration (E_v) rates and other climatological data may be obtained from either data recorded on site or from the Station Climatic Summary for a nearby airport.

Meteorological parameters—such as the evapotranspiration rate and the runoff rate—may also be found in resources such as Geraghty, Miller, van der Leeden, and Troise (1973). Surface runoff may also be estimated by using the curve number equation developed by the U.S. Soil Conservation Service (U.S. EPA 1990a). U.S. EPA (1985b) cites isopleths of mean annual cropland runoff corresponding to various curve numbers developed by Stewart, Woolhiser, Wischmeier, Caro, and Frere (1975). Curve numbers are assigned to an area on the basis of soil type, land use or cover, and the hydrologic condition of the soil (U.S. EPA 1990a).

Using these different references may introduce uncertainties and limitations. For example, Geraghty, van der Leeden, and Troise (1973) present isopleths for annual surface water contributions that include interflow and ground water recharge; these values should be adjusted downward to reflect surface runoff only. U.S. EPA (1994b) recommends that these values be reduced by 50 percent.

Soil Volumetric Water Content (θ_{sw})

The soil volumetric water content θ_{sw} depends on the available water and the soil structure. A wide range of values for these variables may apply in the various U.S. EPA regions. Consistent with earlier guidance documents (U.S. EPA 1994b), U.S. EPA OSW recommends the following value for θ_{sw}.

Recommended Value for: Soil Volumetric Water Content (θ_{sw})
0.2 ml/cm^3 soil

Additional information on soil water content is presented in Appendix B, specific to the equations in which it is used.

3.11.2 CALCULATION OF COPC CONCENTRATIONS IN SURFACE WATER AND SEDIMENTS

COPC concentrations in surface water and sediments are calculated for all water bodies selected for evaluation in the risk assessment. Mechanisms considered for determination of COPC loading of the water column are:

(1) Direct deposition,

(2) Runoff from impervious surfaces within the watershed,

(3) Runoff from pervious surfaces within the watershed,

(4) Soil erosion over the total watershed,

(5) Direct diffusion of vapor phase COPCs into the surface water, and

(6) Internal transformation of compounds chemically or biologically.

Other potential mechanisms may require consideration on a case-by-case basis (e.g., tidal influences), however, contributions from other potential mechanisms are assumed to be negligible in comparison with those being evaluated.

The USLE and a sediment delivery ratio are used to estimate the rate of soil erosion from the watershed. To evaluate the COPC loading to a water body from its associated watershed, the COPC concentration in watershed soils should be calculated. As described in Section 3.11.1, the equation for COPC concentration in soil includes a loss term that considers the loss of contaminants from the soil after deposition. These loss mechanisms may all lower the soil concentration associated with a specific deposition rate.

Surface water concentration algorithms include a sediment mass balance, in which the amount of sediment assumed to be buried and lost from the water body is equal to the difference between the amount of soil introduced to the water body by erosion and the amount of suspended solids lost in downstream flow. As a result, the assumptions are made that sediments do not accumulate in the water body over time, and an equilibrium is maintained between the surficial layer of sediments and the water column. The total water column COPC concentration is the sum of the COPC concentration dissolved in water and the COPC

concentration associated with suspended solids. Partitioning between water and sediment varies with the COPC. The total concentration of each COPC is partitioned between the sediment and the water column.

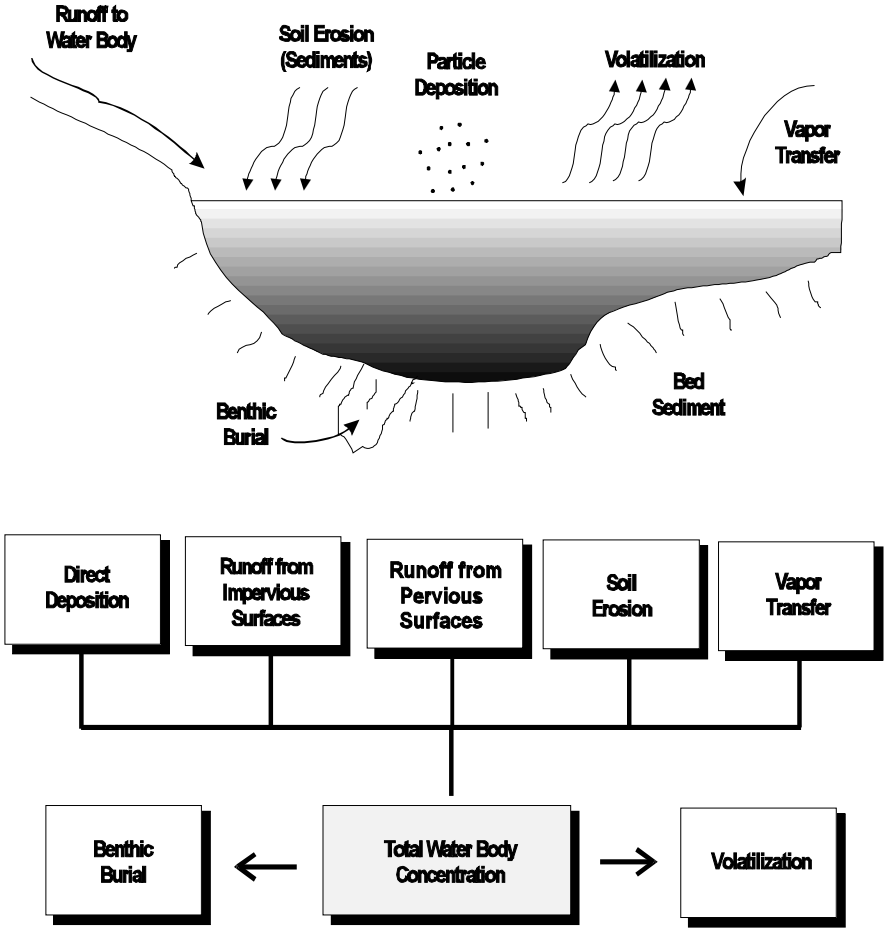


Figure 3-5 COPC Loading to the Water Body

Section 3.11.2.1 describes equations for computing COPC loading to a water body. Section 3.11.2.2 describes equations for computing total COPC concentration in a water body. Section 3.11.2.3 present the equations for computing COPC concentration in water column and in sediment. These equations are also presented and further defined in Appendix B.

3.11.2.1 Total COPC Loading to a Water Body (L_T)

Consistent with earlier U.S. EPA guidance (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-10 to calculate the total COPC load to a water body (L_T). This equation is also further described in Appendix B, Table B-2-1.

Recommended Equation for Calculating:
Total COPC Load to the Water Body (L_T)

$$L_T = L_{DEP} + L_{dif} + L_{RI} + L_R + L_E + L_I \qquad \text{Equation 3-10}$$

where

L_T	=	Total COPC load to the water body (including deposition, runoff, and erosion) (g/yr)
L_{DEP}	=	Total (wet and dry) particle phase and wet vapor phase COPC direct deposition load to water body (g/yr)
L_{dif}	=	Vapor phase COPC diffusion (dry deposition) load to water body (g/yr)
L_{RI}	=	Runoff load from impervious surfaces (g/yr)
L_R	=	Runoff load from pervious surfaces (g/yr)
L_E	=	Soil erosion load (g/yr)
L_I	=	Internal transfer (g/yr)

Due to the limited data and uncertainty associated with the chemical or biological internal transfer, L_I, of compounds into daughter products, U.S. EPA OSW recommends a default value for this variable of zero. However, if a permitting authority determines that site-specific conditions indicate calculation of internal transfer should be considered, U.S. EPA OSW recommends following the methodologies described in U.S. EPA NCEA document, *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (U.S EPA In Press). Calculation of each of the remaining variables (L_{DEP}, L_{dif}, L_{RI}, L_R, and L_E) is discussed in the following subsections.

Total (Wet and Dry) Particle Phase and Wet Vapor Phase Contaminant Direct Deposition Load to Water Body (L_{DEP})

Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends Equation 3-11 to calculate the load to the water body from the direct deposition of wet and dry particles and wet vapors onto the surface of the water body (L_{DEP}). The equation is also further described in Appendix B, Table B-2-2.

Recommended Equation for Calculating:
Total Particle Phase and Wet Vapor Phase Direct Deposition Load to Water Body (L_{DEP})

$$L_{DEP} = Q \cdot [\ F_v \cdot Dywwv + (1 - F_v\ ) \cdot Dytwp\ ] \cdot A_W \qquad \text{Equation 3-11}$$

where

L_{DEP}	=	Total (wet and dry) particle phase and wet vapor phase COPC direct deposition load to water body (g/yr)
Q	=	COPC emission rate (g/s)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
Dywwv	=	Unitized yearly (water body and watershed) average wet deposition from vapor phase (s/m^2-yr)
Dytwp	=	Unitized yearly (water body and watershed) average total (wet and dry) deposition from vapor phase (s/m^2-yr)
A_W	=	Water body surface area (m^2)

Section 3.9 describes the unitized air parameters, *Dywwv* and *Dywwv*, obtained as output from the ISCST3 air dispersion modeling. The determination of water body surface area, A_w, is described in Chapter 4. Appendix A-2 describes determination of the compound-specific parameter, F_v.

Diffusion Load to Water Body (L_{dif})

Consistent with earlier U.S. EPA guidance (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends using Equation 3-12 to calculate the dry vapor phase COPC diffusion load to the water body (L_{dif}). The equation is described in detail in Appendix B, Table B-2-3.

Recommended Equation for Calculating:
Vapor Phase COPC Diffusion (Dry Deposition) Load to Water Body (L_{Dif})

$$L_{dif} = \frac{K_v \cdot Q \cdot F_v \cdot Cywv \cdot A_W \cdot 1 \times 10^{-6}}{\frac{H}{R \cdot T_{wk}}} \qquad \text{Equation 3-12}$$

where

L_{dif}	=	Vapor phase COPC diffusion (dry deposition) load to water body (g/yr)
K_v	=	Overall COPC transfer rate coefficient (m/yr)
Q	=	COPC emission rate (g/s)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
$Cywv$	=	Unitized yearly (water body and watershed) average air concentration from vapor phase (μg-s/g-m^3)
A_W	=	Water body surface area (m^2)
10^{-6}	=	Units conversion factor (g/μg)
H	=	Henry's Law constant (atm-m^3/mol)
R	=	Universal gas constant (atm-m^3/mol-K)
T_{wk}	=	Water body temperature (K)

The overall COPC transfer rate coefficient (K_v) is calculated by using the equation in Appendix B, Table B-2-13. Consistent with previous U.S. EPA guidance (1994l; 1993h) and U.S. EPA (1998c), U.S. EPA OSW recommends a water body temperature (T_{wk}) of 298 K (or 25°C). Section 3.9 describes the determination of the modeled air parameter, *Cywv*. The determination of water body surface area, A_w, is described in Chapter 4. Appendix A-2 describes determination of compound-specific parameters, F_v and H.

Runoff Load from Impervious Surfaces (L_{RI})

In some watershed soils, a fraction of the wet and dry deposition in the watershed will be to impervious surfaces. Dry deposition may accumulate and be washed off during rain events. Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-13 to calculate impervious runoff load to a water body (L_{RI}). The equation is also presented in Appendix B, Table B-2-4.

Recommended Equation for Calculating:
Runoff Load from Impervious Surfaces (L_{RI})

$$L_{RI} = Q \cdot [\ F_v \cdot Dywwv + (1.0 - F_v\ ) \cdot Dytwp\ ] \cdot A_I \qquad \text{Equation 3-13}$$

where

L_{RI}	=	Runoff load from impervious surfaces (g/yr)
Q	=	COPC emission rate (g/s)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
Dywwv	=	Unitized yearly (water body and watershed) average wet deposition from vapor phase (s/m^2-yr)
Dytwp	=	Unitized yearly (water body and watershed) average total (wet and dry) deposition from vapor phase (s/m^2-yr)
A_I	=	Impervious watershed area receiving COPC deposition (m^2)

Impervious watershed area receiving COPC deposition (A_I) is the portion of the total effective watershed area that is impervious to rainfall (i.e., roofs, driveways, streets, and parking lots) and drains to the water body.

Runoff Load from Pervious Surfaces (L_R)

Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-14 to calculate the runoff dissolved COPC load to the water body from pervious soil surfaces in the watershed (L_R). The equation is also presented in Appendix B, Table B-2-5.

Recommended Equation for Calculating:
Runoff Load from Pervious Surfaces (L_R)

$$L_R = RO \cdot (A_L - A_I) \cdot \frac{Cs \cdot BD}{\theta_{sw} + Kd_s \cdot BD} \cdot 0.01 \qquad \text{Equation 3-14}$$

where

L_R	=	Runoff load from pervious surfaces (g/yr)
RO	=	Average annual surface runoff from pervious areas (cm/yr)
A_L	=	Total watershed area receiving COPC deposition (m^2)
A_I	=	Impervious watershed area receiving COPC deposition (m^2)
Cs	=	COPC concentration in soil (in watershed soils) (mg COPC/kg soil)
BD	=	Soil bulk density (g soil/cm^3 soil)
θ_{sw}	=	Soil volumetric water content (mL water/cm^3 soil)
Kd_s	=	Soil-water partition coefficient (cm^3 water/g soil)
0.01	=	Units conversion factor (kg-cm^2/mg-m^2)

Appendix B describes the determination of site-specific parameters, RO, A_L, A_I, BD, and θ_{sw}. The calculation of the COPC concentration in soil (Cs) is discussed in Section 3.11.1 and Appendix B. Soil bulk density (BD) and soil water content (θ_{sw}) are described in Section 3.11.1.4.

Soil Erosion Load (L_E)

Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-15 to calculate soil erosion load (L_E). The equation is also presented in Appendix B, Table B-2-6.

Recommended Equation for Calculating:
Soil Erosion Load (L_E)

$$L_E = X_e \cdot (A_L - A_I) \cdot SD \cdot ER \cdot \frac{Cs \cdot Kd_s \cdot BD}{\theta_{sw} + Kd_s \cdot BD} \cdot 0.001 \qquad \text{Equation 3-15}$$

where

L_E	=	Soil erosion load (g/yr)
X_e	=	Unit soil loss (kg/m^2-yr)
A_L	=	Total watershed area (evaluated) receiving COPC deposition (m^2)
A_I	=	Impervious watershed area receiving COPC deposition (m^2)
SD	=	Sediment delivery ratio (watershed) (unitless)
ER	=	Soil enrichment ratio (unitless)
Cs	=	COPC concentration in soil (in watershed soils) (mg COPC/kg soil)
BD	=	Soil bulk density (g soil/cm^3 soil)
θ_{sw}	=	Soil volumetric water content (mL water/cm^3 soil)
Kd_s	=	Soil-water partition coefficient (mL water/g soil)
0.001	=	Units conversion factor (k-cm^2/mg-m^2)

Unit soil loss (X_e) and watershed sediment delivery ratio (SD) are calculated as described in the following subsections and in Appendix B. COPC concentration in soil (Cs) is described in Section 3.11.1 and Appendix B, Table B-1-1. Soil bulk density (BD) and soil water content (θ_{sw}) are described in Section 3.11.1.4.

Universal Soil Loss Equation - USLE

U.S. EPA OSW recommends that the universal soil loss equation (USLE), Equation 3-16, be used to calculate the unit soil loss *(X_e)* specific to each watershed. This equation is further described in Appendix B, Table B-2-7. Appendix B also describes determination of the site- and watershed-specific values for each of the variables associated with Equation 3-16. The use of Equation 3-16 is consistent with U.S. EPA (1994b; 1994l) and U.S. EPA (1998c).

Recommended Equation for Calculating:
Unit Soil Loss (X_e)

$$X_e = RF \cdot K \cdot LS \cdot C \cdot PF \cdot \frac{907.18}{4047} \qquad \text{Equation 3-16}$$

where

X_e	=	Unit soil loss (kg/m^2-yr)
RF	=	USLE rainfall (or erosivity) factor (yr^{-1})
K	=	USLE erodibility factor (ton/acre)
LS	=	USLE length-slope factor (unitless)
C	=	USLE cover management factor (unitless)
PF	=	USLE supporting practice factor (unitless)
907.18	=	Units conversion factor (kg/ton)
4047	=	Units conversion factor (m^2/acre)

The USLE *RF* variable, which represents the influence of precipitation on erosion, is derived from data on the frequency and intensity of storms. This value is typically derived on a storm-by-storm basis, but average annual values have been compiled (U.S. Department of Agriculture 1982). Information on determining site-specific values for variables used in calculating X_e is provided in U.S. Department of Agriculture (U.S. Department of Agriculture 1997) and U.S. EPA guidance (U.S. EPA 1985b). Refer to Appendix B, Table B-2-7 for additional discussion of the USLE.

Sediment Delivery Ratio (*SD*)

U.S. EPA OSW recommends the use of Equation 3-17 to calculate sediment delivery ratio (*SD*). The use of this equation is further described in Appendix B, Table B-2-8.

Recommended Equation for Calculating:
Sediment Delivery Ratio *(SD)*

$$SD = a \cdot (A_L)^{-b} \qquad \text{Equation 3-17}$$

where

SD	=	Sediment delivery ratio (watershed) (unitless)
a	=	Empirical intercept coefficient (unitless)
b	=	Empirical slope coefficient (unitless)
A_L	=	Total watershed area (evaluated) receiving COPC deposition (m^2)

The sediment delivery ratio (*SD*) for a large land area, a watershed or part of a watershed, can be calculated, on the basis of the area of the watershed, by using an approach proposed by Vanoni (1975). Accordingly, U.S. EPA (1993h) recommended the use of Equation 3-17 to calculate the sediment delivery ratio.

According to Vanoni (1975), sediment delivery ratios vary approximately with the -0.125 power of the drainage area. Therefore, the empirical slope coefficient is assumed to be equal to 0.125. An inspection of the data presented by Vanoni (1975) indicates that the empirical intercept coefficient varies with the size of the watershed, as illustrated in Appendix B, Table B-2-8.

A_L is the total watershed surface area affected by deposition that drains to the body of water. A watershed includes all of the land area that contributes water to a water body. In assigning values to the watershed surface area affected by deposition, consideration should be given to (1) the distance from the stack, (2) the location of the area affected by deposition fallout with respect to the water body, and (3) in the absence of

any deposition considerations, watershed hydrology. Total sediment in a water body may have originated from watershed soils that are (or have the potential to be) both affected and unaffected by deposition of combustion emissions. If a combustor is depositing principally on a land area that feeds a tributary of a larger river system, consideration must be given to an "effective" area. An effective drainage area will almost always be less than the watershed.

3.11.2.2 Total Water Body COPC Concentration (C_{wtot})

U.S. EPA OSW recommends the use of Equation 3-18 to calculate total water body COPC concentration (C_{wtot}). The total water body concentration includes both the water column and the bed sediment. The equation is also presented in Appendix B, Table B-2-9.

Recommended Equation for Calculating:
Total Water Body COPC Concentration (C_{wtot})

$$C_{wtot} = \frac{L_T}{Vf_x \cdot f_{wc} + k_{wt} \cdot A_W \cdot (d_{wc} + d_{bs})} \qquad \text{Equation 3-18}$$

where

C_{wtot}	=	Total water body COPC concentration (including water column and bed sediment) (g COPC/m^3 water body)
L_T	=	Total COPC load to the water body (including deposition, runoff, and erosion) (g/yr)
Vf_x	=	Average volumetric flow rate through water body (m^3/yr)
f_{wc}	=	Fraction of total water body COPC concentration in the water column (unitless)
k_{wt}	=	Overall total water body COPC dissipation rate constant (yr^{-1})
A_W	=	Water body surface area (m^2)
d_{wc}	=	Depth of water column (m)
d_{bs}	=	Depth of upper benthic sediment layer (m)

The total COPC load to the water body (L_T)—including deposition, runoff, and erosion—is described in Section 3.11.2.1 and Appendix B, Table B-2-1. The depth of the upper benthic layer (d_{bs}), which represents the portion of the bed that is in equilibrium with the water column, cannot be precisely specified;

however, U.S. EPA (1993h) recommended values ranging from 0.01 to 0.05. Consistent with U.S. EPA (1994l; 1998c), U.S. EPA OSW recommends a default value of 0.03, which represents the midpoint of the specified range. Issues related to the remaining parameters are summarized in the following subsections.

Fraction of Total Water Body COPC Concentration in the Water Column (f_{wc}) and Benthic Sediment (f_{bs})

Consistent with U.S. EPA (1998c), U.S. EPA OSW recommends using Equation 3-19 to calculate fraction of total water body COPC concentration in the water column (f_{wc}), and Equation 3-20 to calculate fraction of total water body contaminant concentration in benthic sediment (f_{bs}). The equations are also presented in Appendix B, Table B-2-10.

Recommended Equation for Calculating:
Fraction of Total Water Body COPC Concentration in the Water Column (f_{wc}) and Benthic Sediment (f_{bs})

$$f_{wc} = \frac{(1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}) \cdot d_{wc} / d_z}{(1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}) \cdot d_{wc} / d_z + (\theta_{bs} + Kd_{bs} \cdot BS) \cdot d_{bs} / d_z} \quad \text{Equation 3-19}$$

$$f_{bs} = 1 - f_{wc} \quad \text{Equation 3-20}$$

where

f_{wc}	=	Fraction of total water body COPC concentration in the water column (unitless)
f_{bs}	=	Fraction of total water body COPC concentration in benthic sediment (unitless)
Kd_{sw}	=	Suspended sediments/surface water partition coefficient (L water/kg suspended sediment)
TSS	=	Total suspended solids concentration (mg/L)
1×10^{-6}	=	Units conversion factor (kg/mg)
d_z	=	Total water body depth (m)
θ_{bs}	=	Bed sediment porosity ($L_{water}/L_{sediment}$)

Kd_{bs}	=	Bed sediment/sediment pore water partition coefficient (L water/kg bottom sediment)
BS	=	Benthic solids concentration (g/cm^3 [equivalent to kg/L])
d_{wc}	=	Depth of water column (m)
d_{bs}	=	Depth of upper benthic sediment layer (m)

U.S. EPA (1993h) and NC DEHNR (1997) recommended the use of Equations 3-19 and 3-20 to calculate the fraction of total water body concentration occurring in the water column (f_{wc}) and the bed sediments (f_{bs}). The partition coefficient Kd_{sw} describes the partitioning of a contaminant between sorbing material, such as soil, surface water, suspended solids, and bed sediments (see Appendix A-2). NC DEHNR (1997) also recommended adding the depth of the water column to the depth of the upper benthic layer ($d_{wc} + d_{bs}$) to calculate the total water body depth (d_z).

NC DEHNR (1997) recommended a default total suspended solids (*TSS*) concentration of 10 mg/L, which was adapted from U.S. EPA (1993h). However, due to variability in water body specific values for this variable, U.S. EPA OSW recommends the use of water body-specific measured *TSS* values representative of long-term average annual values for the water body of concern. Average annual values for *TSS* are generally expected to be in the range of 2 to 300 mg/L; with additional information on anticipated *TSS* values available in the U.S. EPA NCEA document, *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (U.S. EPA In Press).

If measured data is not available, or of unacceptable quality, a calculated *TSS* value can be obtained for non-flowing water bodies using Equation 3-21.

$$TSS = \frac{X_e \cdot (A_L - A_I) \cdot SD \cdot 1x10^3}{Vf_x + D_{ss} \cdot A_W} \qquad \text{Equation 3-21}$$

where

TSS	=	Total suspended solids concentration (mg/L)
X_e	=	Unit soil loss (kg/m^2-yr)
A_L	=	Total watershed area (evaluated) receiving COPC deposition (m^2)
A_I	=	Impervious watershed area receiving COPC deposition (m^2)

SD	=	Sediment delivery ratio (watershed) (unitless)
Vf_x	=	Average volumetric flow rate through water body (value should be 0 for quiescent lakes or ponds) (m^3/yr)
D_{ss}	=	Suspended solids deposition rate (a default value of 1,825 for quiescent lakes or ponds) (m/yr)
A_W	=	Water body surface area (m^2)

The default value of 1,825 m/yr provided for D_{ss} is characteristic of Stoke's settling velocity for an intermediate (fine to medium) silt.

Also, to evaluate the appropriateness of watershed-specific values (specific for non-flowing water bodies) used in calculating the unit soil loss (X_e), as described in Section 3.11.2.1 and Appendix B, the water-body specific measured *TSS* value should be compared to the calculated *TSS* value obtained using Equation 3-21. If the measured and calculated *TSS* values differ significantly, parameter values used in calculating X_e should be re-evaluated. This re-evaluation of *TSS* and X_e should also be conducted if the calculated *TSS* value is outside of the normal range expected for average annual measured values, as discussed above.

Bed sediment porosity (θ_{bs}) can be calculated from the benthic solids concentration by using the following equation (U.S. EPA 1993h):

$$\theta_{bs} = 1 - \frac{BS}{\rho_s}$$

where

θ_{bs}	=	Bed sediment porosity ($L_{water}/L_{sediment}$)
ρ_s	=	Bed sediment density (kg/L)
BS	=	Benthic solids concentration (kg/L)

U.S. EPA OSW recommends the following default value for bed sediment porosity (θ_{bs}), which was adapted from U.S. EPA (1993h) and U.S. EPA (1998c):

Recommended Value for:
Bed Sediment Porosity (θ_{bs})

$$\theta_{bs} = 0.6 \ L_{water}/L_{sediment}$$

(assuming ρ_s = 2.65 kg/L [bed sediment density] and BS = 1 kg/L [benthic solids concentration])

Values for the benthic solids concentration (BS) and depth of upper benthic sediment layer (d_{bs}) range from 0.5 to 1.5 kg/L and 0.01 to 0.05 meters, respectively. However, consistent with earlier U.S. EPA guidance (1993h; 1994l) and U.S. EPA (1998c), 1 kg/L is a reasonable default for most applications of the benthic solids concentration (BS), and 0.03 meter is the default depth of the upper benthic layer (d_{bs}). The default depth of 0.03 meters is based on the midpoint of the range presented above. The use of this equation is further described in Appendix B, Table B-2-10.

Overall Total Water Body COPC Dissipation Rate Constant (k_{wt})

Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-22 to calculate the overall dissipation rate of COPCs in surface water, resulting from volatilization and benthic burial. The equation is also presented in Appendix B, Table B-2-11.

Recommended Equation for Calculating:
Overall Total Water Body COPC Dissipation Rate Constant (k_{wt})

$$k_{wt} = f_{wc} \cdot k_v + f_{bs} \cdot k_b \qquad \text{Equation 3-22}$$

where

k_{wt}	=	Overall total water body dissipation rate constant (yr^{-1})
f_{wc}	=	Fraction of total water body COPC concentration in the water column (unitless)
k_v	=	Water column volatilization rate constant (yr^{-1})
f_{bs}	=	Fraction of total water body COPC concentration in benthic sediment (unitless)
k_b	=	Benthic burial rate constant (yr^{-1})

The variables f_{wc} and f_{bs} are discussed in the previous section, Equations 3-19 and 3-20, and calculated by using the equations presented in Appendix B, Table B-2-10.

Water Column Volatilization Rate Constant (k_v)

Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends using Equation 3-23 to calculate water column volatilization rate constant. The equation is also presented in Appendix B, Table B-2-12.

Recommended Equation for Calculating:
Water Column Volatilization Rate Constant (k_v)

$$k_v = \frac{K_v}{d_z \cdot (1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6})} \qquad \text{Equation 3-23}$$

where

k_v	=	Water column volatilization rate constant (yr^{-1})
K_v	=	Overall COPC transfer rate coefficient (m/yr)
d_z	=	Total water body depth (m)
Kd_{sw}	=	Suspended sediments/surface water partition coefficient (L water/kg suspended sediments)
TSS	=	Total suspended solids concentration (mg/L)
1×10^{-6}	=	Units conversion factor (kg/mg)

Total water body depth (d_z), suspended sediment and surface water partition coefficient (Kd_{sw}), and total suspended solids concentration (TSS), are previously described in this section. Kd_{sw} is discussed in Appendix A-2. The overall transfer rate coefficient (K_v) is described in the following subsection.

Overall COPC Transfer Rate Coefficient (K_v)

Volatile organic chemicals can move between the water column and the overlying air. The overall transfer rate K_v, or conductivity, is determined by a two-layer resistance model that assumes that two "stagnant

films" are bounded on either side by well-mixed compartments. Concentration differences serve as the driving force for the water layer diffusion. Pressure differences drive the diffusion for the air layer. From balance considerations, the same mass must pass through both films; the two resistances thereby combine in series, so that the conductivity is the reciprocal of the total resistance.

Consistent with U.S. EPA (1993h) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-24 to calculate the overall transfer rate coefficient (K_v). The equation is also presented in Appendix B, Table B-2-13.

Recommended Equation for Calculating:
Overall COPC Transfer Rate Coefficient (K_v)

$$K_v = \left(K_L^{-1} + \left(K_G \cdot \frac{H}{R \cdot T_{wk}} \right)^{-1} \right)^{-1} \cdot \theta^{T_{wk} - 293} \qquad \text{Equation 3-24}$$

where

K_v	=	Overall COPC transfer rate coefficient (m/yr)
K_L	=	Liquid phase transfer coefficient (m/yr)
K_G	=	Gas phase transfer coefficient (m/yr)
H	=	Henry's Law constant (atm-m^3/mol)
R	=	Universal gas constant (atm-m^3/mol-K)
T_{wk}	=	Water body temperature (K)
θ	=	Temperature correction factor (unitless)

The value of the conductivity K_v depends on the intensity of turbulence in the water body and the overlying atmosphere. As Henry's Law constant increases, the conductivity tends to be increasingly influenced by the intensity of turbulence in water. Conversely, as Henry's Law constant decreases, the value of the conductivity tends to be increasingly influenced by the intensity of atmospheric turbulence.

The liquid and gas phase transfer coefficients, K_L and K_G, respectively, vary with the type of water body. The liquid phase transfer coefficient (K_L) is calculated by using Equations 3-25 and 3-26. The gas phase transfer coefficient (K_G) is calculated by using Equations 3-27 and 3-28.

Henry's Law constants generally increase with increasing vapor pressure of a COPC and generally decrease with increasing solubility of a COPC. Henry's Law constants are compound-specific and are presented in Appendix A-2. The universal ideal gas constant, R, is 8.205×10^{-5} atm-m^3/mol-K, at 20°C. The temperature correction factor (θ), which is equal to 1.026, is used to adjust for the actual water temperature. Volatilization is assumed to occur much less readily in lakes and reservoirs than in moving water bodies.

Liquid Phase Transfer Coefficient (K_L)

Consistent with U.S. EPA (1998c), U.S. EPA OSW recommends using Equations 3-25 and 3-26 to calculate liquid phase transfer coefficient. (K_L). The use of these equations is further described in Appendix B, Table B-2-14.

Recommended Equation for Calculating:
Liquid Phase Transfer Coefficient (K_L)

For flowing streams or rivers:

$$K_L = \sqrt{\frac{(1 \times 10^{-4}) \cdot D_w \cdot u}{d_z}} \cdot 3.1536 \times 10^7 \qquad \text{Equation 3-25}$$

For quiescent lakes or ponds:

$$K_L = (C_d^{0.5} \cdot W) \cdot \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \cdot \frac{k^{0.33}}{\lambda_z} \cdot \left(\frac{\mu_w}{\rho_w \cdot D_w}\right)^{-0.67} \cdot 3.1536 \times 10^7 \qquad \text{Equation 3-26}$$

where

K_L	=	Liquid phase transfer coefficient (m/yr)
D_w	=	Diffusivity of COPC in water (cm^2/s)
u	=	Current velocity (m/s)
1×10^{-4}	=	Units conversion factor (m^2/cm^2)
d_z	=	Total water body depth (m)
C_d	=	Drag coefficient (unitless)
W	=	Average annual wind speed (m/s)

ρ_a	=	Density of air (g/cm^3)
ρ_w	=	Density of water (g/cm^3)
k	=	von Karman's constant (unitless)
λ_z	=	Dimensionless viscous sublayer thickness (unitless)
μ_w	=	Viscosity of water corresponding to water temperature (g/cm-s)
3.1536 x 10^7	=	Units conversion factor (s/yr)

For a flowing stream or river, the transfer coefficients are controlled by flow-induced turbulence. For these systems, the liquid phase transfer coefficient is calculated by using Equation 3-25, which is the O'Connor and Dobbins (1958) formula, as presented in U.S. EPA (1993h).

For a stagnant system (quiescent lake or pond), the transfer coefficient is controlled by wind-induced turbulence. For quiescent lakes or ponds, the liquid phase transfer coefficient can be calculated by using Equation 3-26 (O'Connor 1983; U.S. EPA 1993h).

The total water body depth (d_z) for liquid phase transfer coefficients is discussed previously in this section.

Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of the following default values. These values are further described in Appendix A-2:

(1) a diffusivity of chemical in water ranging (D_w) from 1.0×10^{-5} to 8.5×10^{-2} cm^2/s,

(2) a dimensionless viscous sublayer thickness (λ_z) of 4,

(3) a von Karman's constant (k) of 0.4,

(4) a drag coefficient (C_d) of 0.0011 which was adapted from U.S. EPA (1993h),

(5) a density of air (ρ_a) of 0.0012 g/cm^3 at standard conditions (temperature = 20°C or 293 K, pressure = 1 atm or 760 millimeters of mercury) (Weast 1986),

(6) a density of water (ρ_w) of 1 g/cm^3 (Weast 1986),

(7) a viscosity of water (μ_w) of a 0.0169 g/cm-s corresponding to water temperature (Weast 1986).

Gas Phase Transfer Coefficient (K_G)

U.S. EPA OSW recommends using Equations 3-27 and 3-28 to calculate gas phase transfer coefficient (K_G). The equation is also discussed in Appendix B, Table B-2-15.

Recommended Equation for Calculating:
Gas Phase Transfer Coefficient (K_G)

For flowing streams or rivers:

$$K_G = 36500 \text{ m/yr} \qquad \text{Equation 3-27}$$

For quiescent lakes or ponds:

$$K_G = (C_d^{0.5} \cdot W) \cdot \frac{k^{0.33}}{\lambda_z} \cdot \left(\frac{\mu_a}{\rho_a \cdot D_a}\right)^{-0.67} \cdot 3.1536 \times 10^7 \qquad \text{Equation 3-28}$$

where

K_G	=	Gas phase transfer coefficient (m/yr)
C_d	=	Drag coefficient (unitless)
W	=	Average annual wind speed (m/s)
k	=	von Karman's constant (unitless)
λ_z	=	Dimensionless viscous sublayer thickness (unitless)
μ_a	=	Viscosity of air corresponding to air temperature (g/cm-s)
ρ_a	=	Density of air corresponding to water temperature (g/cm^3)
D_a	=	Diffusivity of COPC in air (cm^2/s)
3.1536 x 10^7	=	Units conversion factor (s/yr)

U.S. EPA (1993h) indicated that the rate of transfer of a COPC from the gas phase for a flowing stream or river is assumed to be constant, in accordance with O'Connor and Dobbins (1958) (Equation 3-27).

For a stagnant system (quiescent lake or pond), the transfer coefficients are controlled by wind-induced turbulence. For quiescent lakes or ponds, U.S. EPA OSW recommends that the gas phase transfer coefficient be computed by using the equation presented in O'Connor (1983) (Equation 3-28).

Consistent with U.S. EPA (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends 1.81 x 10^{-4} g/cm-s for the viscosity of air corresponding to air temperature.

Benthic Burial Rate Constant (k_b)

U.S. EPA OSW recommends using Equation 3-29 to calculate benthic burial rate (k_b). The equation is also discussed in Appendix B, Table B-2-16.

Recommended Equation for Calculating:
Benthic Burial Rate Constant (k_b)

$$k_b = \left(\frac{X_e \cdot A_L \cdot SD \cdot 1 \times 10^3 - Vf_x \cdot TSS}{A_W \cdot TSS} \right) \cdot \left(\frac{TSS \cdot 1 \times 10^{-6}}{BS \cdot d_{bs}} \right) \qquad \text{Equation 3-29}$$

where

k_b	=	Benthic burial rate constant (yr^{-1})
X_e	=	Unit soil loss (kg/m^2-yr)
A_L	=	Total watershed area (evaluated) receiving deposition (m^2)
SD	=	Sediment delivery ratio (watershed) (unitless)
Vf_x	=	Average volumetric flow rate through water body (m^3/yr)
TSS	=	Total suspended solids concentration (mg/L)
A_W	=	Water body surface area (m^2)
BS	=	Benthic solids concentration (g/cm^3)
d_{bs}	=	Depth of upper benthic sediment layer (m)
1 x 10^{-6}	=	Units conversion factor (kg/mg)
1 x 10^3	=	Units conversion factor (g/kg)

The benthic burial rate constant (k_b), which is calculated in Equation 3-29, can also be expressed in terms of the rate of burial (Wb):

$$Wb = k_b \cdot d_{bs} \qquad \text{Equation 3-30}$$

where

Wb	=	Rate of burial (m/yr)
k_b	=	Benthic burial rate constant (yr^{-1})
d_{bs}	=	Depth of upper benthic sediment layer (m)

According to U.S. EPA (1994l) and U.S. EPA (1998c), COPC loss from the water column resulting from burial in benthic sediment can be calculated by using Equation 3-29. These guidance documents also recommend a benthic solids concentration (*BS*) value ranging from 0.5 to 1.5 kg/L, which was adapted from U.S. EPA (1993h). U.S. EPA OSW recommends the following default value for benthic solids concentration (*BS*).

Recommended Default Value for: Benthic Solids Concentration (*BS*)
1.0 kg/L

The calculated value for k_b should range from 0 to 1.0; with low k_b values expected for water bodies characteristic of no or limited sedimentation (rivers and fast flowing streams), and k_b values closer to 1.0 expected for water bodies characteristic of higher sedimentation (lakes). This range of values is based on the relation between the benthic burial rate and rate of burial expressed in Equation 3-30; with the depth of upper benthic sediment layer held constant. For k_b values calculated as a negative (water bodies with high average annual volumetric flow rates in comparison to watershed area evaluated), a k_b value of 0 should be assigned for use in calculating the total water body COPC concentration (C_{wtot}) in Equation 3-18. If the calculated k_b value exceeds 1.0, re-evaluation of the parameter values used in calculating X_e should be conducted.

3.11.2.3 Total COPC Concentration in Water Column (C_{wctot})

U.S. EPA OSW recommends using Equation 3-31 to calculate total COPC concentration in water column (C_{wctot}). The equation is also discussed in Appendix B, Table B-2-17.

Recommended Equation for Calculating:
Total COPC Concentration in Water Column (C_{wctot})

$$C_{wctot} = f_{wc} \cdot C_{wtot} \cdot \frac{d_{wc} + d_{bs}}{d_{wc}} \qquad \text{Equation 3-31}$$

where

C_{wctot}	=	Total COPC concentration in water column (mg COPC/L water column)
f_{wc}	=	Fraction of total water body COPC concentration in the water column (unitless)
C_{wtot}	=	Total water body COPC concentration, including water column and bed sediment (mg COPC/L water body)
d_{wc}	=	Depth of water column (m)
d_{bs}	=	Depth of upper benthic sediment layer (m)

The use of Equation 3-31 to calculate total COPC concentration in water column is consistent with U.S. EPA (1994l; 1998c).

Total water body COPC concentration—including water column and bed sediment (C_{wtot}) and fraction of total water body COPC concentration in the water column (f_{wc})—should be calculated by using Equation 3-18 and Equation 3-19, respectively. Depth of upper benthic sediment layer (d_{bs}) is discussed previously.

Dissolved Phase Water Concentration (C_{dw})

U.S. EPA OSW recommends the use of Equation 3-32 to calculate the concentration of COPC dissolved in the water column (C_{dw}). The equation is discussed in detail in Appendix B, Table B-2-18.

Recommended Equation for Calculating:
Dissolved Phase Water Concentration (C_{dw})

$$C_{dw} = \frac{C_{wctot}}{1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}} \qquad \text{Equation 3-32}$$

where

C_{dw}	=	Dissolved phase water concentration (mg COPC/L water)
C_{wctot}	=	Total COPC concentration in water column (mg COPC/L water column)
Kd_{sw}	=	Suspended sediments/surface water partition coefficient (L water/kg suspended sediment)
TSS	=	Total suspended solids concentration (mg/L)
1×10^{-6}	=	Units conversion factor (kg/mg)

The use of Equation 3-32 to calculate the concentration of COPC dissolved in the water column is consistent with U.S. EPA (1994l; 1998c).

The total COPC concentration in water column (C_{wctot}) is calculated by using the Equation 3-31 (see also Appendix B, Table B-2-17). The surface water partition coefficient (Kd_{sw}) and total suspended solids concentration (*TSS*) are discussed previously.

COPC Concentration in Bed Sediment (*Csed*)

U.S. EPA OSW recommends the use of Equation 3-33 to calculate COPC concentration in bed sediment (*Csed*). The equation is also presented in Appendix B, Table B-2-19.

Recommended Equation for Calculating:
COPC Concentration in Bed Sediment (*Csed*)

$$C_{sed} = f_{bs} \cdot C_{wtot} \cdot \left(\frac{Kd_{bs}}{\theta_{bs} + Kd_{bs} \cdot BS} \right) \cdot \left(\frac{d_{wc} + d_{bs}}{d_{bs}} \right) \qquad \text{Equation 3-33}$$

where

C_{sed}	=	COPC concentration in bed sediment (mg COPC/kg sediment)
f_{bs}	=	Fraction of total water body COPC concentration in benthic sediment (unitless)
C_{wtot}	=	Total water body COPC concentration, including water column and bed sediment (mg COPC/L water body)
Kd_{bs}	=	Bed sediment/sediment pore water partition coefficient (L COPC/kg water body)
θ_{bs}	=	Bed sediment porosity ($L_{pore\ water}/L_{sediment}$)
BS	=	Benthic solids concentration (g/cm^3)
d_{wc}	=	Depth of water column (m)
d_{bs}	=	Depth of upper benthic sediment layer (m)

The use of Equation 3-33 to calculate the COPC concentration in bed sediment is consistent with U.S. EPA (1994l; 1998c).

The total water body COPC concentration—including water column and bed sediment (C_{wtot}) and the fraction of total water body COPC concentration that occurs in the benthic sediment (f_{bs})—is calculated by using Equations 3-18 and 3-20, respectively. The bed sediment and sediment pore water partition coefficient (Kd_{bs}) is discussed in Appendix A-2. Bed sediment porosity (θ_{bs}), benthic solids concentration (BS), depth of water column (d_{wc}), and depth of upper benthic layer (d_{bs}) are discussed previously.

3.11.3 CALCULATION OF COPC CONCENTRATIONS IN PLANTS

The concentration of COPCs in plants is assumed to occur by three possible mechanisms:

- **Direct deposition of particles—**wet and dry deposition of particle phase COPCs onto the exposed plant surfaces.
- **Vapor transfer—**uptake of vapor phase COPCs by plants through their foliage.

- **Root uptake—**root uptake of COPCs available from the soil and their transfer to the aboveground portions of the plant.

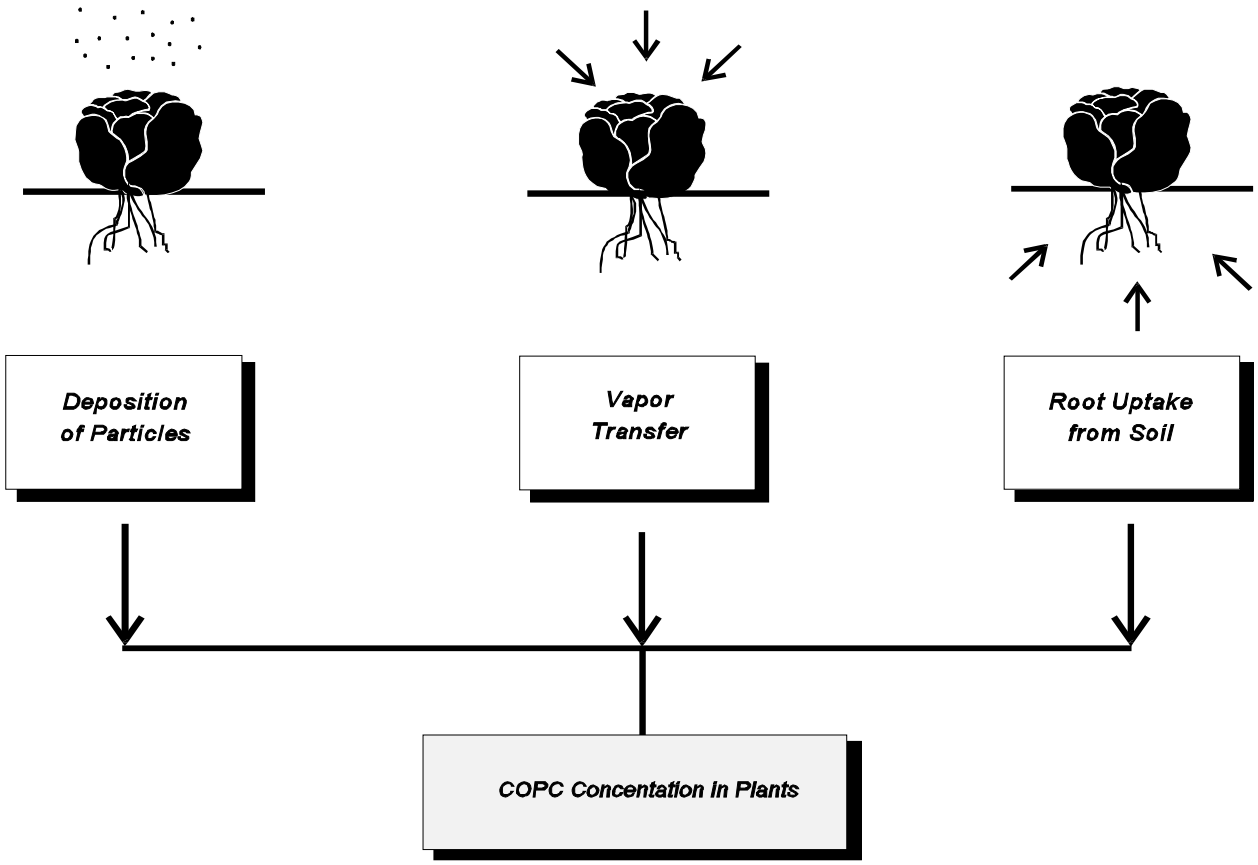


Figure 3-6 COPC Concentration in Plants

The total COPC concentration in terrestrial plants, C_{TP} is calculated as a sum of contamination occurring through all three of these mechanisms.

3.11.3.1 Calculating Plant Concentration Due to Direct Deposition (*Pd*)

Consitent with previous U.S. EPA guidance (1994l) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-34 to calculate COPC concentration in plants due to direct deposition. The use of this equation is further described in Appendix B, Table B-3-1.

Recommended Equation for Calculating:
Plant Concentration Due to Direct Deposition (*Pd*)

$$Pd = \frac{1{,}000 \cdot Q \cdot (1 - Fv) \cdot [Dydp + (Fw \cdot Dywp)] \cdot Rp \cdot [1.0 - \exp(-kp \cdot Tp)] \cdot 0.12}{Yp \cdot kp} \quad \text{Equation 3-34}$$

where

Pd	=	Plant concentration due to direct (wet and dry) deposition (mg COPC/kg WW)
1,000	=	Units conversion factor (mg/g)
Q	=	COPC emission rate (g/s)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
Dydp	=	Unitized yearly average dry deposition from particle phase (s/m^2-yr)
Fw	=	Fraction of COPC wet deposition that adheres to plant surfaces (unitless)
Dywp	=	Unitized yearly wet deposition from particle phase (s/m^2-yr)
Rp	=	Interception fraction of the edible portion of plant (unitless)
kp	=	Plant surface loss coefficient (yr^{-1})
Tp	=	Length of plant exposure to deposition per harvest of the edible portion of the *i*th plant group (yr)
012	=	Dry weight to wet weight conversion factor (unitless)
Yp	=	Yield or standing crop biomass of the edible portion of the plant (productivity) (kg DW/m^2)

Section 3.9 describes the use of the unitized air parameters, *Dydp* and *Dywp*, obtained as output from the air dispersion modeling. Appendix A-3 describes determination of *Fv*. Appendix B describes determination of *Fw*, *Rp*, *kp*, *Tp*, and *Yp*. The dry weight to wet weight conversion factor of 0.12 is based on the average rounded value from the range of 80 to 95 percent water content in herbaceous plants and nonwoody plant parts (Taiz at al. 1991).

3.11.3.2 Calculating Plant Concentration Due to Air-to-Plant Transfer (*Pv*)

Consistent with U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-35 to calculate the plant concentration due to air-to-plant transfer (*Pv*). The use of this equation is further described in Appendix B, Table B-3-2.

Recommended Equation for Calculating:
Plant Concentration Due to Air-to-Plant Transfer (*Pv*)

$$Pv = Q \cdot F_v \cdot 0.12 \cdot \frac{Cyv \cdot Bv}{\rho_a} \qquad \text{Equation 3-35}$$

where

Pv	=	Plant concentration due to air-to-plant transfer (mg COPC/kg WW)
Q	=	COPC emission rate (g/s)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
Cyv	=	Unitized yearly average air concentration from vapor phase (μg-s/g-m^3)
Bv	=	Air-to-plant biotransfer factor ([mg COPC/g DW plant]/[mg COPC/g air]) (unitless)
012	=	Dry weight to wet weight conversion factor (unitless)
ρ_a	=	Density of air (g/m^3)

Section 3.9 describes the use of the unitized air parameter, *Cyv*. Appendix A-3 describes determination of the COPC-specific parameters, *Fv* and *Bv*. The dry weight to wet weight conversion factor of 0.12 is based on the average rounded value from the range of 80 to 95 percent water content in herbaceous plants and nonwoody plant parts (Taiz at al. 1991). Appendix B further describes use of Equation 3-35, including determination of *Fw* and ρ_a.

3.11.3.3 Calculating Plant Concentration Due to Root Uptake (*Pr*)

Consistent with previous U.S. EPA guidance (1994g; 1994l; 1995h) and U.S. EPA (1998c), U.S. EPA OSW recommends the use of Equation 3-36 to calculate the plant concentration due to root uptake (*Pr*). The use of this equation is further described in Appendix B, Table B-3-3.

Recommended Equation for Calculating:
Plant Concentration Due to Root Uptake (*Pr*)

$$Pr = Cs \cdot BCF_r \cdot 0.12 \qquad \text{Equation 3-36}$$

where

Pr	=	Plant concentration due to root uptake (mg COPC/kg WW)
BCF_r	=	Plant-soil biotransfer factor (unitless)
Cs	=	COPC concentration in soil (mg COPC/kg soil)
012	=	Dry weight to wet weight conversion factor (unitless)

Equation 3-36 is based on the soil-to-aboveground plant transfer approach developed by Travis and Arms (1988). The dry weight to wet weight conversion factor of 0.12 is based on the average rounded value from the range of 80 to 95 percent water content in herbaceous plants and nonwoody plant parts (Taiz at al. 1991). Appendix A-3 describes determination of the COPC-specific parameter BCF_r. Section 3.11.1 and Appendix B describe calculation of *Cs*.

3.12 REPLACING DEFAULT PARAMETER VALUES

As discussed in Chapter 1, default parameter values are provided in this guidance for numerous inputs to the fate and transport modeling. After completing a risk assessment based on the default parameter values recommended in this guidance, risk assessors may choose to investigate replacing default parameter values with measured or published values if a more representative estimate of site-specific risk can be obtained. Use of parameter values other than those specified in this guidance should always be clearly described in the risk assessment report and work plan, and approved by the permitting authority. U.S. EPA OSW recommends that requests to change default parameter values include the following information, as appropriate:

1. An explanation of why the use of a measured or published value other than the default value is warranted (e.g., the default parameter value is based on data or studies at sites in the northwestern U.S., but the facility is located in the southeast);

2. The supporting technical basis of the replacement parameter value, including readable copies (printed in English) of any relevant technical literature or studies;

3. The basis of the default parameter value, as understood by the requestor, including readable copies (printed in English) of the referenced literature or studies (if available);

4. A comparison of the weight-of-evidence between the competing studies (e.g., the proposed replacement parameter value is based on a study that is more representative of site conditions, a specific exposure setting being evaluated, or a more scientifically valid study than the default parameter value, the proposed replacement parameter is based on the analysis of 15 samples as opposed to 5 for the default parameter value, or the site-specific study used more stringent quality control/quality assurance procedures than the study upon which the default parameter value is based);

5. A description of other risk assessments or projects where the proposed replacement parameter value has been used, and how such risk assessments or projects are similar to the risk assessment in consideration.

Chapter 4
Problem Formulation

What's Covered in Chapter 4:

- Exposure Setting Characterization
- Food Web Development
- Selecting Assessment Endpoints
- Identifying Measures of Effect

Problem formulation establishes the exposure setting used as the basis for exposure analysis and risk characterization. Problem formulation includes (1) characterization of the exposure setting for identification of potentially exposed habitats in the assessment area (Section 4.1); (2) development of food webs representative of the habitats to be evaluated (Section 4.2); (3) selection of assessment endpoints relevant to food web structure and function (Section 4.3); and (4) identification of measurement receptors (Section 4.4).

4.1 EXPOSURE SETTING CHARACTERIZATION

Exposure setting characterization is important in the identification of habitats consisting of ecological receptors in the assessment area that may be impacted as a result of exposure to compounds emitted from a facility. Ecological receptors within a potentially impacted habitat can be evaluated through consideration of the combination of exposure pathways to which ecological receptors representing a habitat-specific food web may be exposed to a compound. The habitats identified to be evaluated are selected based on existing habitats surrounding the facility (see Section 4.1.1); and also support which habitat-specific food webs are evaluated in risk characterization. Consideration of ecological receptors representative of the habitats also provides the basis for selecting measurement receptors, as well as, it supports demonstration of the presence or absence of federal and state species of special interest (see Section 4.1.1.3).

Exposure setting characterization is generally focused geographically to the assessment area that is defined as the area surrounding the facility that is impacted from facility emissions as predicted by ISCST3 air dispersion modeling; with additional consideration typically extending by a 50-km radius, taken from the centroid of a polygon (also used as the origin of ISCST3 receptor grid node array, see Chapter 3) identified by the UTM coordinates of the facility's emission sources. A 50-km radius is generally the recognized limit of the ISCST3 air dispersion model and its predecessors (U.S. EPA 1990a; 1995c). Resources for characterizing the exposure setting should focus on the areas impacted from emissions as predicted by air dispersion modeling. As discussed in Section 4.1.1, habitats (potentially including water bodies and their associated watersheds)—both within and outside the facility property boundary—should be considered for evaluation.

The following subsections provide information on selection of habitats, and identification of ecological receptors representative of those habitats, to be considered for evaluation in the risk assessment.

4.1.1 Selection of Habitats

Habitats to be considered in the risk assessment are selected by identifying similar habitats surrounding the facility that are potentially impacted by facility emissions, and when overlayed with the air dispersion modeling results, define which habitat-specific food webs should be evaluated in the risk assessment. Habitats can be defined based on their biotic and abiotic characteristics, and are generally divided into two major groups (i.e., terrestrial and aquatic) that can be classified as follows:

- Terrestrial
  - Forest
  - Shortgrass praire
  - Tallgrass praire
  - Agricultural/Cropland
  - Scrub/Shrub
  - Desert
- Aquatic
  - Freshwater
  - Brackish/Intermediate
  - Marine

Habitat types can typically be identified by reviewing hard copy and/or electronic versions of land use land classification (LULC) maps, topographic maps, and aerial photographs. Sources and general information associated with each of these data types or maps are presented below. Also, as noted in Chapter 3, the UTM coordinate system format (NAD27 or NAD83) for all mapping information should be verified to ensure consistency and prevent erroneous georeferencing of locations and areas.

Land Use Land Cover (LULC) Maps - LULC maps can be downloaded directly from the USGS web site (http://mapping.usgs.gov./index.html), at a scale of 1:250,000 in a file type GIRAS format. LULC maps can also be downloaded from the EPA web site (ftp://ftp.epa.gov/pub), at a scale of 1:250,000, in an Arc/Info export format. These maps provide detailed habitat information based upon the classification system and definitions of Level II Land Use and Land Cover information. Exact boundaries of polygon land use area coverages, in areas being considered for evaluation, should be verified using available topographic maps and aerial photographic coverages.

Topographic Maps - Topographic maps are readily available in both hard copy and electronic format directly from USGS or numerous other vendors. These maps are commonly at a scale of 1:24,000, and in a file type of TIFF format with TIFF World File included for georeferencing.

Aerial Photographs - Hard copy aerial photographs can be purchased directly form USGS in a variety of scales and coverages. Electronic format aerial photographs of Digital Ortho Quarter Quads (DOQQs) can also be purchased directly form USGS, or from an increasing number of commercial sources. Properly georeferenced DOQQs covering a 3-km or more radius of the assessment area, overlays of the LULC map coverage, and the ISCST3 modeled receptor grid node array provide an excellent reference for identifying land use areas and justifying selection of exposure locations.

While these data types or maps do not represent the universe of information available on habitats or land use, they are readily available from a number of governmental sources (typically accessible via the Internet), usually can be obtained free or for a low cost, and, when used together, provide sufficient information to reliably identify and define boundaries of habitats to be considered for evaluation in risk characterization. However, while the use of these or other data can be very accurate, verifying identified habitats by conducting a site visit is recommended. Also, these data sources may be dated, and may not reflect current habitat boundaries or land use (i.e., expanded cropland or urban developments, new lakes).

Additional information useful for habitat identification can be obtained from discussions with representatives of private and government organizations which routinely collect and evaluate ecosystem or habitat information including the following: (1) Soil Conservation Service, (2) U.S. Fish and Wildlife

Service (FWS), (3) U.S Department of Agriculture, (4) state natural resource, wildlife, and park agencies, and (5) local government agencies.

U.S. EPA OSW recommends that habitats identified during exposure setting characterization and selected for evaluation in the risk assessment be clearly mapped and include the following supporting information:

- Facility boundaries
- Facility emission source location(s)
- Habitat types and boundaries
- Water bodies and their asssociated watersheds
- Special ecological areas (see Section 4.1.1.2)

A facility location map, including land-use and land cover data, which allows for identification of habitats to support selection of habitat-specific food webs to be evaluated in the risk assessment. The map should also note the UTM coordinate system format (NAD27 or NAD83) for all information presented to ensure consistency and prevent erroneous georeferencing of locations and areas; including accurate identification of exposure scenario locations and water bodies within the habitat to be evaluated, as discussed in the following subsections.

4.1.1.1 Selection of Exposure Scenario Locations Within Terrestrial Habitats

Exposure scenario locations to be evaluated within the terrestrial habitats identified during the exposure setting characterization, are selected at specific receptor grid nodes based on evaluation of the magnitude of air parameter values estimated by ISCST3 (see Chapter 3). U.S. EPA OSW would like to note that the methodology and resulting selection of receptor grid nodes as exposure scenario locations is one of the most critical parts of the risk assessment process, ensuring standardization across all facilities evaluated and reproducibility of results. The estimates of risk can vary significantly in direct response to the receptor grid nodes that are selected as exposure scenario locations because the grid node-specific ISCST3 modeled air parameter values are used as inputs into the media equations.

U.S. EPA OSW recommends that, at a minimum, the procedures described below be used in the selection of receptor grid nodes as exposure scenario locations; and that the selected exposure scenario locations correspond to actual ISCST3 modeled receptor grid node locations defined by UTM coordinates. In addition to consistency and reproducibility, these procedures ensure that the exposure scenario location(s) selected for evaluation over a specified habitat do not overlook the most highly impacted locations. Exposure scenario locations, at actual receptor grid nodes, should be selected as follows:

Step 1: Define Terrestrial Habitats To Be Evaluated - All habitats, identified during exposure setting characterization for evaluation in the risk assessment, should be defined and habitat boundaries mapped in a format (NAD 27 or NAD 83 UTM) consistent with that used to define locations of facility emission sources and modeld ISCST3 receptor grid nodes.

Step 2: Identify Receptor Grid Node(s) Within Each Habitat To Be Evaluated - For each habitat to be evaluated, identify the receptor grid nodes within that area or on the boundary of that area (defined in Step 1) that represent the locations of highest yearly average concentration for each ISCST3 modeled air parameter (i.e., air concentration, dry deposition, wet deposition) for each phase (i.e., vapor, particle, particle-bound). This determination should be performed for each emission source (i.e., stacks, fugitives) and all emissions sources at the facility combined. This results in the selection of one or more receptor grid nodes as exposure scenario locations, within a defined habitat area to be evaluated, and that meet one or more of the following criteria:

- Highest modeled unitized vapor phase air concentration
- Highest modeled unitized vapor phase wet deposition rate
- Highest modeled unitized particle phase air concentration
- Highest modeled unitized particle phase wet deposition rate
- Highest modeled unitized particle phase dry deposition rate
- Highest modeled unitized particle-bound phase air concentration
- Highest modeled unitized particle-bound phase wet deposition rate
- Highest modeled unitized particle-bound phase dry deposition rate

Only ISCST3 modeled air parameters corresponding to a single receptor grid node should be used per exposure scenario location as inputs into the media equations, without averaging or statistical manipulation. However, based generally on the number and location of facility emission sources, multiple exposure scenario locations may be selected to represent the highest potential impact area for a specific habitat being evaluated.

Modeling of the above air parameter criteria for habitats at actual sites being evaluated in U.S. EPA Region 6, using actual modeled air parameters, indicates that only 1 to 3 receptor nodes are typically selected per habitat. This is because, in most cases, the location of some of the highest air concentration and deposition rate, within a habitat for several of the modeled air parameters, occurs at the same receptor grid node. The number of receptor grid nodes with maximum air parameters depends on many factors, including number of and distance between emissions sources, habitat size and shape, distance and direction from facility, topographic features, and meteorological patterns. It should also be noted, that while these criteria minimize overlooking maximum risk within a habitat, they do not preclude the risk assessor from selecting additional exposure scenario locations within that same habitat based on site-specific risk considerations.

Also, a water body and associated watershed in close proximity to the exposure scenario location being evaluated should be identified to represent a drinking water source for applicable receptors (see Appendix F). Although the locations and type of sources (i.e., free water, consumption of water as part of food items) of water ingested by an animal through diet are expected to vary depending on the receptor and availability, COPC intake by the receptor through ingestion of water can be estimated by assuming only water intake from a defined water body for which a COPC concentration can be calculated. Therefore, a representative water body should be defined and evaluated following the guidance provided in Section 4.1.1.2, and a COPC concentration in the water column, C_{wctot}, calculated as described in Chapter 3 and Appendix B.

If a definable water body is not located within or in close proximity to the terrestrial habitat being evaluated, receptor drinking water intake terms in the exposure equations presented in Appendix F should be adjusted accordingly (i.e., ingestion of drinking water set equal to zero). However, for sites where the permitting authority or risk manager identifies that receptor exposure through ingestion of drinking water may be significant, an available option is to assume that a small water body exists at the same receptor grid node as the exposure scenario location being evaluated. If multiple exposure scenario locations within the habitat are being evaluated, a single assumed water body can be located at the closest receptor grid node located equal distance from each of the exposure scenario locations being evaluated, and utilized as a drinking water source for evaluation of each exposure scenario location within the habitat. Since the assumed water body represents a pool or other drinking source too small for identification on an aerial

photograph or map, it can be assumed to have a unit volume (i.e., surface area of 1 meter square, water column depth of 1 meter). The assumed water body should not have flow or an associated watershed.

4.1.1.2 Selection of Habitat Exposure Scenrario Locations Within Aquatic Habitats

Exposure scenario locations to be evaluated within the aquatic habitats identified during the exposure setting characterization may first require differentiating water bodies from land areas within aquatic habitiats not typically covered by water (e.g., flood plains or wetland areas transitioning to terrestrial and upland habitats). Exposure scenario locations within land areas of aquatic habitats not characteristic of a standing water body are selected following the same steps as for terrestrial habitats (see Section 4.1.1.1). However, exposure scenario locations for defined water bodies within aquatic habitats should be selected following the guidance provided in this section. The associated watershed contributing COPC loading to the water body being evaluated should also be defined.

U.S. EPA OSW recommends that, at a minimum, the following procedures be used in the selection of exposure scenario locations within defined water body areas of aquatic habitats as follows:

> ***Step 1: Define Aquatic Habitats To Be Evaluated -*** All habitats, identified during exposure setting characterization for evaluation in the risk assessment, should be defined and habitat boundaries mapped in a format (NAD 27 or NAD 83 UTM) consistent with that used to define locations of facility emission sources and modeled ISCST3 receptor grid nodes. Water body boundaries should reflect annual average shoreline elevations. The area extent of watersheds associated with water bodies to be evaluated should also be defined.
>
> ***Step 2: Identify Receptor Grid Node(s) Within Each Habitat To Be Evaluated -*** For each water body and associated watershed to be evaluated, the receptor grid nodes within that area and on the boundary of that area (defined in Step 1) should be considered. For water bodies, the risk assessor can select the receptor grid node that represent the locations of highest yearly average concentration for each ISCST3 modeled air parameter (i.e., air concentration, dry deposition, wet deposition) for each phase (i.e., vapor, particle, particle-bound), or average the air parameter values for all receptor grid nodes within the area of the water body. This determination should be performed for each emission source (i.e., stacks, fugitives), and all emissions sources at the facility combined. For watersheds, the modeled air parameter values should be averaged for all receptor grid nodes within the area extent or effective area of the watershed (excluding the area of the water body).

For evaluating the COPC loading to the water body from its associated watershed, the area extent of the watershed should be defined and the ISCST3 modeled air parameter values at each receptor grid node

within the watershed area (excluding the water body) averaged. These averaged air parameter values are then used in the estimating media equations presented in Chapter 3 and Appendix B for calculating the COPC loading to the water body.

For water bodies identified as potentially impacted from emission sources and selected for evaluation, the area extent of the associated watershed that contributes water to the water body should also be identified and defined by UTM coordinates. The area extent of a watershed is generally defined by topographic highs that result in downslope drainage into the water body. The watershed can be important to determining the overall water body COPC loading, because pervious and impervious areas of the watershed, as well as the soil concentration of COPCs resulting from emissions from facility sources, are also used in the media concentration equations to calculate the water body COPC concentrations resulting from watershed runoff (see Chapter 3 and Appendix B). The total watershed area that contributes water to the water body can be very extensive relative to the area that is impacted from facility emissions. Therefore, it is important that the area extent of all watersheds to be evaluated should be approved by the permitting authority, to ensure that the watershed and its contribution to the water body is defined appropriately in consideration of the aquatic habitat being evaluated and subsequent estimated risk.

For example, if facility emissions impact principally a land area that feeds a specific tributary that drains to a large swamp system and immediately upstream of the ISCST3 receptor grid nodes identified as exposure scenario locations for the aquatic habitat defined by the swamp, the risk assessor should consider evaluating an "effective" watershed area rather than the entire watershed area of the large swamp system. For such a large swamp system, the watershed area can be on the order of thousands of square kilometers and can include numerous tributaries draining into the swamp at points that would have no net impact on the water body COPC concentration at the exposure point(s) of interest.

Similar to large watersheds, water bodies may also be extensive in size relative to the area that is impacted from facility emissions and exposure point(s) of interest. In such cases, the risk assessor should consider defining and evaluating an "effective" area of the water body that focuses the assessment specific to areas potentially impacted and of most concern when considering potential for exposure. Therefore, as with watersheds, it is important that the area extent of all water bodies to be evaluated should be approved by the permitting authority, to ensure that potential impacts and exposure are appropriately considered.

The recommended ISCST3 modeled receptor grid node array extends out about 10 km from facility emission sources (see Chapter 3). To address evaluation of habitat areas, water bodies, or watersheds located beyond the coverage provided by the recommended receptor grid node array (greater than 10 km from the facility), the ISCST3 modeling can be conducted with an additional receptor grid node array specified to provide coverage of the area of concern, or the steps above can be executed using the closest receptor grid nodes from the recommended array. However, using the closest receptor grid nodes from the recommended receptor grid node array will in most cases provide a conservative estimate of risk since the magnitude of air parameter values at these receptor grid nodes would most likely be higher than at receptor grid nodes located further from the facility sources and actually within the area of concern.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT

- Identification and/or mapping of habitats, water bodies, and associated watersheds potentially impacted by facility emissions of COPCs, including surface area of the water body and area extent of the contributing watershed defined by UTM coordinates
- Rational for selection or exclusion from evaluation, habitats within the assessment area
- Description of rational and assumptions made to limit the watershed area to an "effective" area
- Copies of all maps, photographs, or figures used to define characteristics of habitats, water bodies, and watersheds

4.1.1.3 Special Ecological Areas

A special ecological area is a habitat that could require protection or special consideration on a site-specific basis because (1) unique and/or rare ecological receptors and natural resources are present, or (2) legislatively-conferred protection (e.g., a national monument) has been established. All potentially exposed special ecological areas in the assessment area should be identified for consideration. The following are examples of special ecological habitats (U.S. EPA 1997c):

- Marine Sanctuaries
- National river reaches
- Spawning areas critical for maintenance of fish/shellfish species

- Terrestrial areas utilized for breeding by large or dense aggregations of animals
- Migratory pathways and feeding areas critical for maintenance of anadromous fish species
- National Preserves
- Federal lands designated for protection of natural ecosystems
- National or State Wildlife Refuges
- Critical areas identified under the Clean Lakes Program
- Habitats known to be used by Federal or State designated or proposed endangered or threatened species
- Areas identified under the Coastal Zone Management Act
- Sensitive areas identified under the National Estuary Program or Near Coastal Waters Program
- Designated Federal Wilderness Areas
- State lands designated for wildlife or game management
- Federal- or State-designated Scenic or Wild Rivers, or Natural Areas
- Wetlands

RECOMMENDED INFORMATION FOR RISK ASSESSMENT

- Identification and mapping of habitats in the assessment area, information on which the identification is based, and information on any special ecological areas. Maps, photographs, or additional sources used to determine habitats and define boundaries should be referenced. Maps and figures should also note the UTM coordinate system format (NAD27 or NAD83) for all information presented to ensure consistency and prevent erroneous georeferencing of locations and areas.

4.1.2 Identification of Ecological Receptors

Identification of ecological receptors during exposure setting characterization is used to define food webs specific to potentially impacted habitats to be evaluated in the risk assessment. Ecological receptors for each habitat potentially impacted should be identified to ensure (1) plant and animal communities representative of the habitat are represented by the habitat-specific food web, and (2) potentially complete exposure pathways are identified. Examples of sources and general information available for identification of site-specific ecological receptors are presented below:

Government Organizations - U.S. Fish and Wildlife Service (National Wetland Inventory Maps - http://nwi.fws.gov) and State Natural Heritage Programs (see Appendix H) provide maps or lists

of species based on geographic location, and are very helpful in identifying threatened or endangered species or areas of special concern.

General Literature (field guides) **-** Examples of information describing the flora and fauna of North America and useful in the development of habitat-specific food webs (see Section 4.2) include the following: Wharton 1982; Craig et al. 1987; Baker et al. 1991; Carr 1994; Ehrlich et al. 1988; National Geographic Society (1987, 1992); Whitaker 1995; Burt and Grossenheider 1980; Behler 1995; Smith and Brodie 1982; Tyning 1990; and Farrand Jr. 1989.

Private or Local Organizations **-** Additional private or professional organizations that are examples of sources of information include: National Audubon Society, National Geographic Society, Local Wildlife Clubs, State and National Parks Systems, and Universities.

Ecological receptor identification should include species both known and expected to be present in a specific habitat being evaluated, and include resident and migratory populations. Identification of flora should be based on major taxonomic groups represented in the assessment area. Natural history information may also be useful during food web development in assigning individual receptors to specific habitats and guilds based on feeding behavior (as discussed in Section 4.2.).

4.2 FOOD WEB DEVELOPMENT

Information obtained during exposure setting characterization should be used to develop one or more habitat-specific food web(s) that represent communities and guilds of receptors potentially exposed to emissions from facility sources. Food webs are interlocking patterns of food chains, which are the straight-line transfer of energy from a food source (e.g., plants) to a series of organisms feeding on the source or on other organisms feeding on the food source (Odum 1971). While energy and, therefore, transfer of a compound in a food chain, is not always linear, it is assumed in this guidance that energy and, thus, compounds, are always transferred to a higher trophic level. The importance of a food chain as an exposure pathway primarily depends on receptor dietary habits, the receptors in the food chain, and other factors including bioavailability and depuration of the compound evaluated.

Habitat-specific food webs are developed for use in the risk assessment to:

- Define direct and indirect exposure pathways
- Formulate assessment endpoints

- Develop mathematical relationships between guilds
- Perform quantitative exposure analysis for ecological receptors

Food webs can be developed using the "community approach" (Cohen 1978), which includes (1) identification of potential receptors in a given habitat (see Section 4.1.2) for grouping into feeding guilds by class and communities (see Section 4.2.1), (2) organizing food web structure by trophic level (e.g., primary producer, secondary consumer; see Section 4.2.2), and (3) defining dietary relationships between guilds and communities (see Section 4.2.3). The result is a complete food web for a defined habitat, which should be developed for each habitat in the assessment area to be evaluated in risk characterization. An example of food web development is presented in Section 4.2.4.

4.2.1 Grouping Receptors into Feeding Guilds and Communities

The first step in developing a habitat-specific food web is to identify, based on the dietary habits and feeding strategies of receptors compiled in Section 4.1.2, the major feeding guilds for birds, mammals, reptiles, amphibians, and fish. A guild is a group of species that occupies a particular trophic level and shares similar feeding strategies. Invertebrates and plants are not assigned to guilds, rather these receptors are grouped into their respective community by the environmental media they inhabit. The distinction for grouping upper-trophic-level receptors into class-specific guilds, and invertebrates and plants into communities, is made because the risk to these groups is characterized differently (see Chapter 5).

Once the major feeding guilds are identified (e.g., herbivore, omnivore, carnivore, insectivore), receptors should be grouped by class (e.g., mammals, birds, amphibians and reptiles, and fish). As noted, invertebrates and plants are grouped into their respective community by the media they inhabit (i.e, soil invertebrates, terrestrial vegetation, sediment fauna, water column invertebrates, phytoplankton, and rooted aquatic vegetation).

4.2.2 Organizing Food Web Structure By Trophic Level

The structure of a food web should be organized by trophic level. A trophic level is one of the successive levels of nourishment in a food web or food chain. The first trophic level (TL1) contains the primary producers or the green plants. Members of this trophic level produce their own food from nutrients,

sunlight, carbon dioxide, and water. These primary producers are also the source of food for members of the second trophic level (TL2). The second trophic level is often refered to as the primary consumers and is composed of animals that eat plants (herbivores) and animals that subsist on detritus (decaying organic matter) found in sediment and soil (detritivores). The third trophic level (TL3), contains both omnivores and carnivores. Omnivores are animals that eat both plant and animal matter, while carnivores eat primarily animal matter. The fourth trophic level (TL4), contains only carnivores and is sometimes refered to as the dominant carnivores. TL4 contains animals at the top of the food chain (e.g., raptorial birds).

Some species can occupy more than one trophic level at a time depending on life stage. For this reason, professional judgement should be used to categorize receptors without making the food web unduly complex.

4.2.3 Defining Dietary Relationships Between Guilds and Communities

After species have been grouped into the appropriate guilds and communities, and organized by trophic level, dietary relationships between guilds and communities should be defined. Guilds and communities should be linked together based on dietary relationships by evaluating the dietary composition of the receptors for each guild and community. Although most organisms have a complex diet, it should be assumed that the majority of their diet is composed of a limited number of prey items and, therefore, a limited number of feeding guild interactions occur. Therefore, U.S. EPA OSW recommends that generally only those interactions that contribute more than five percent of the total diet should be considered for development of a food web. This recommendation of five percent of the total diet as a general cutoff is based on the assumption that the food web can be simplified without underestimating exposure.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT

- Habitat-specific food web(s) that include identification of (1) media (e.g., soil, sediment, water), (2) trophic levels that include at a minimium producers (TL 1), primary consumers (TL 2), secondary consumers (TL 3), and carnivores (TL 4), (3) guilds divided into classes (e.g., herbivorous mammals, omnivorous birds) and communities, and (4) major dietary interactions.

4.2.4 Example Habitat-Specific Food Webs

To better illustrate food web development as discussed in the previous sections (see Sections 4.2.1 through 4.2.3), seven habitat-specific example food webs are presented as Figures 4-1 through 4-7. The habitats represented include:

- Forest
- Tallgrass prairie
- Shortgrass prairie
- Shrub/Scrub
- Freshwater/Wetland
- Salt marsh
- Brackish/Intermediate marsh

The terrestrial and aquatic example food webs are based on information describing the flora and fauna of North America (U.S. FWS 1979; Wharton 1982; Craig et al. 1987; Baker et al. 1991). Supplemental information was collected from field guides and U.S. EPA's *Wildlife Exposure Factors Handbook* (Carr 1994; Ehrlich et al. 1988; National Geographic Society 1987; U.S. EPA 1993o; Whitaker 1995; Burt and Grossenheider 1980; Behler 1995; Smith and Brodie 1982; Tyning 1990; National Geographic Society 1992; Farrand Jr. 1989).

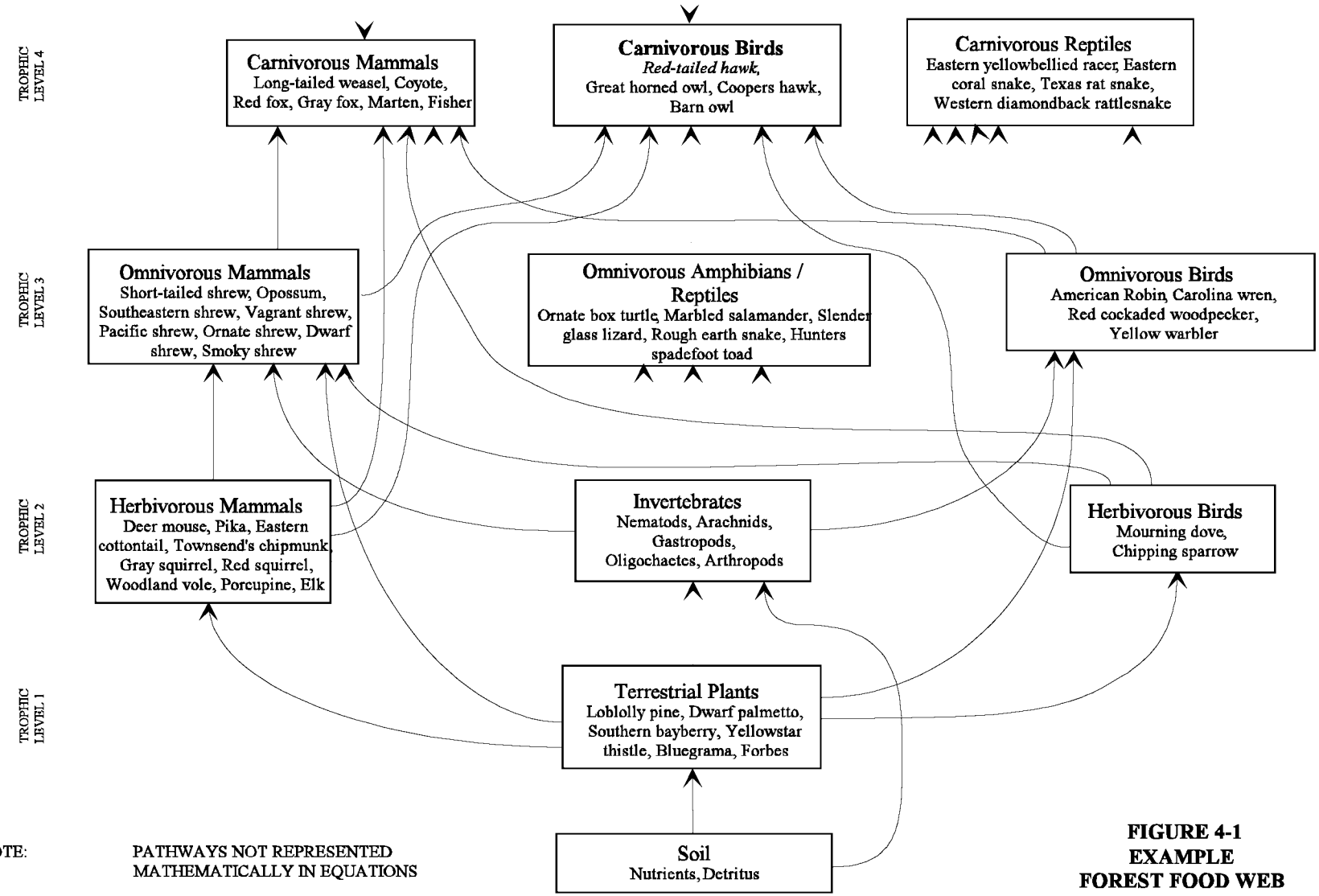


FIGURE 4-1
EXAMPLE
FOREST FOOD WEB

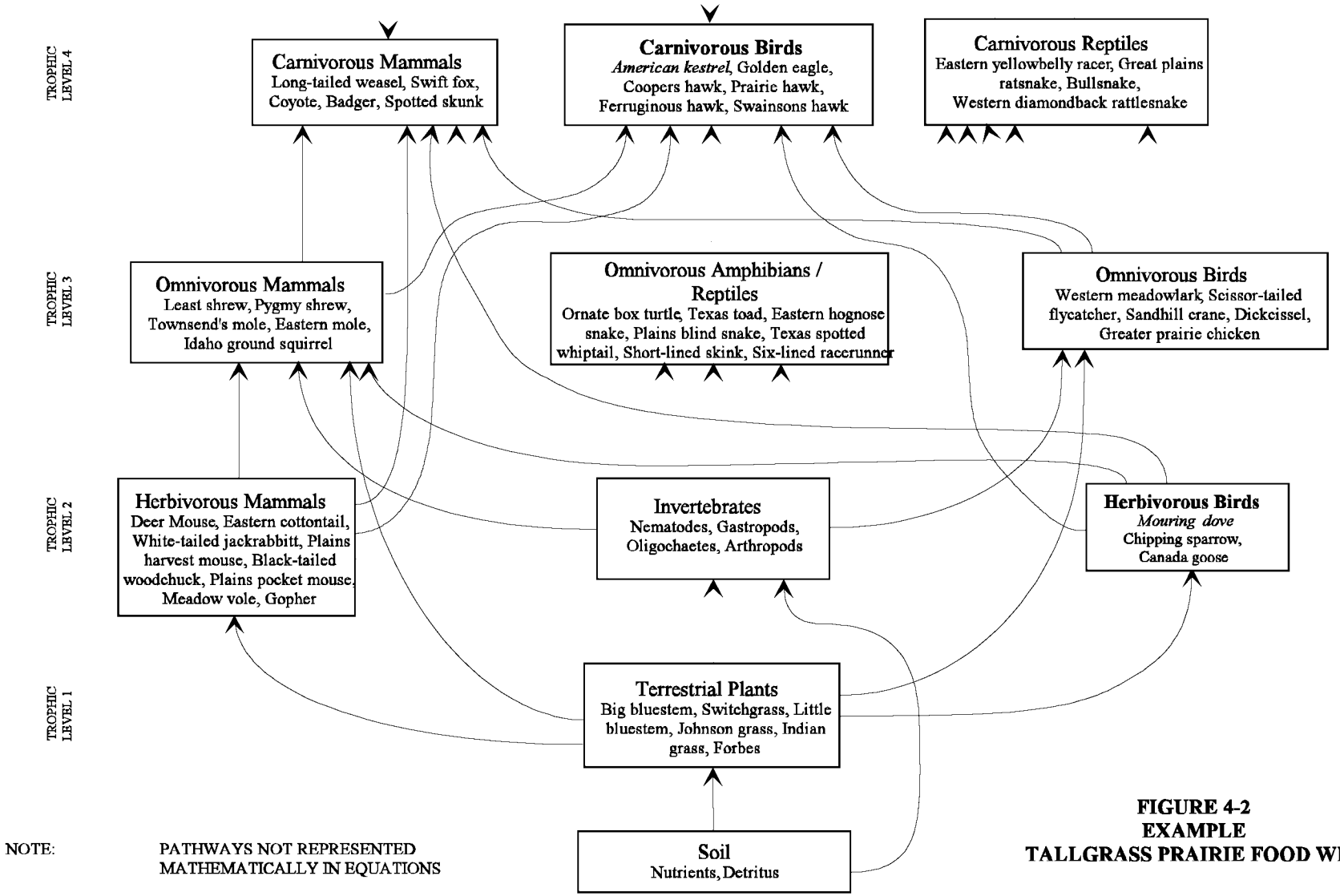
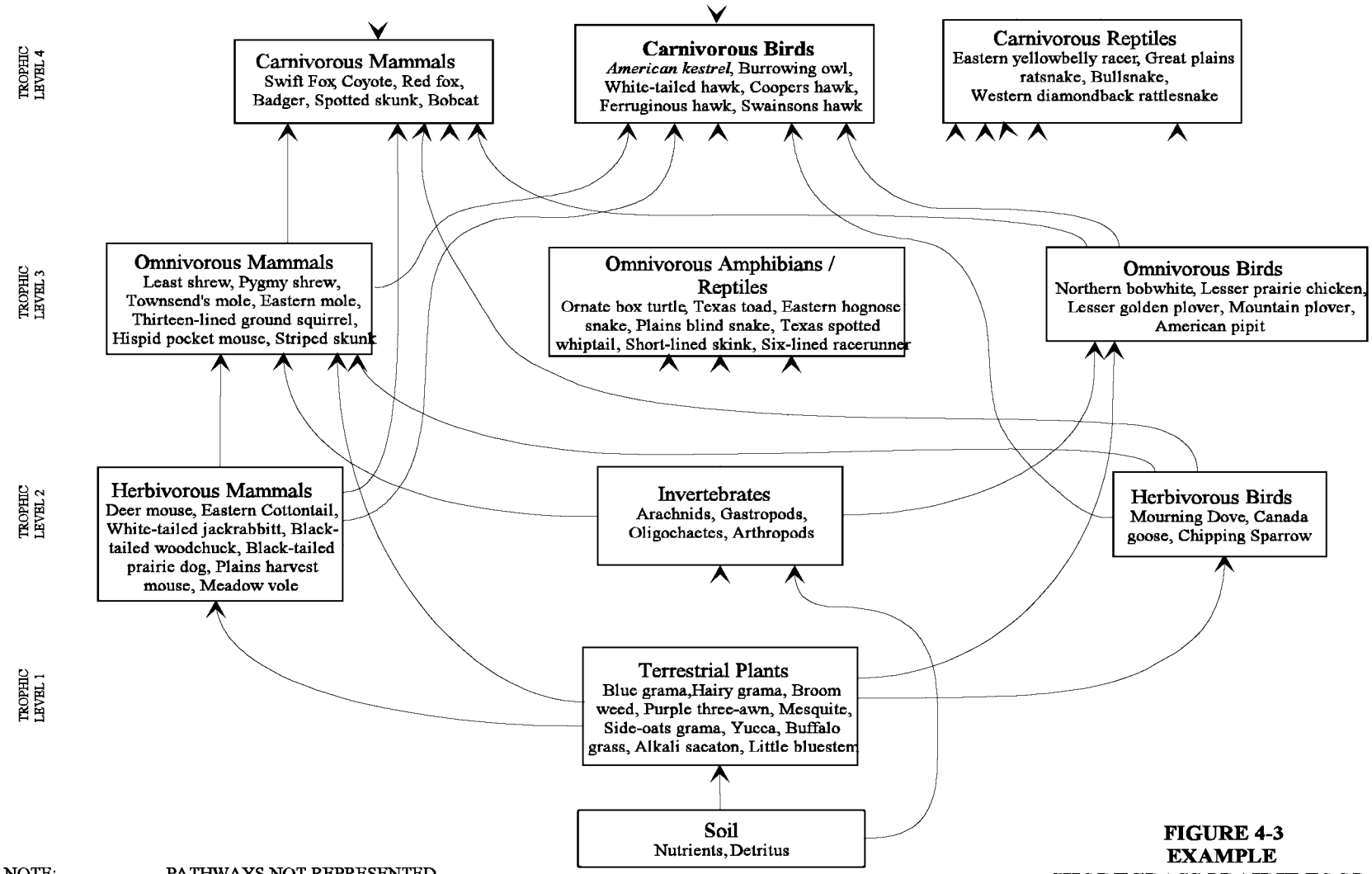


FIGURE 4-2
EXAMPLE
TALLGRASS PRAIRIE FOOD WEB



NOTE: PATHWAYS NOT REPRESENTED MATHEMATICALLY IN EQUATIONS

RECEPTORS LISTED IN ITALICS ARE MEASUREMENT RECEPTORS

FIGURE 4-3
EXAMPLE
SHORTGRASS PRAIRIE FOOD WEB

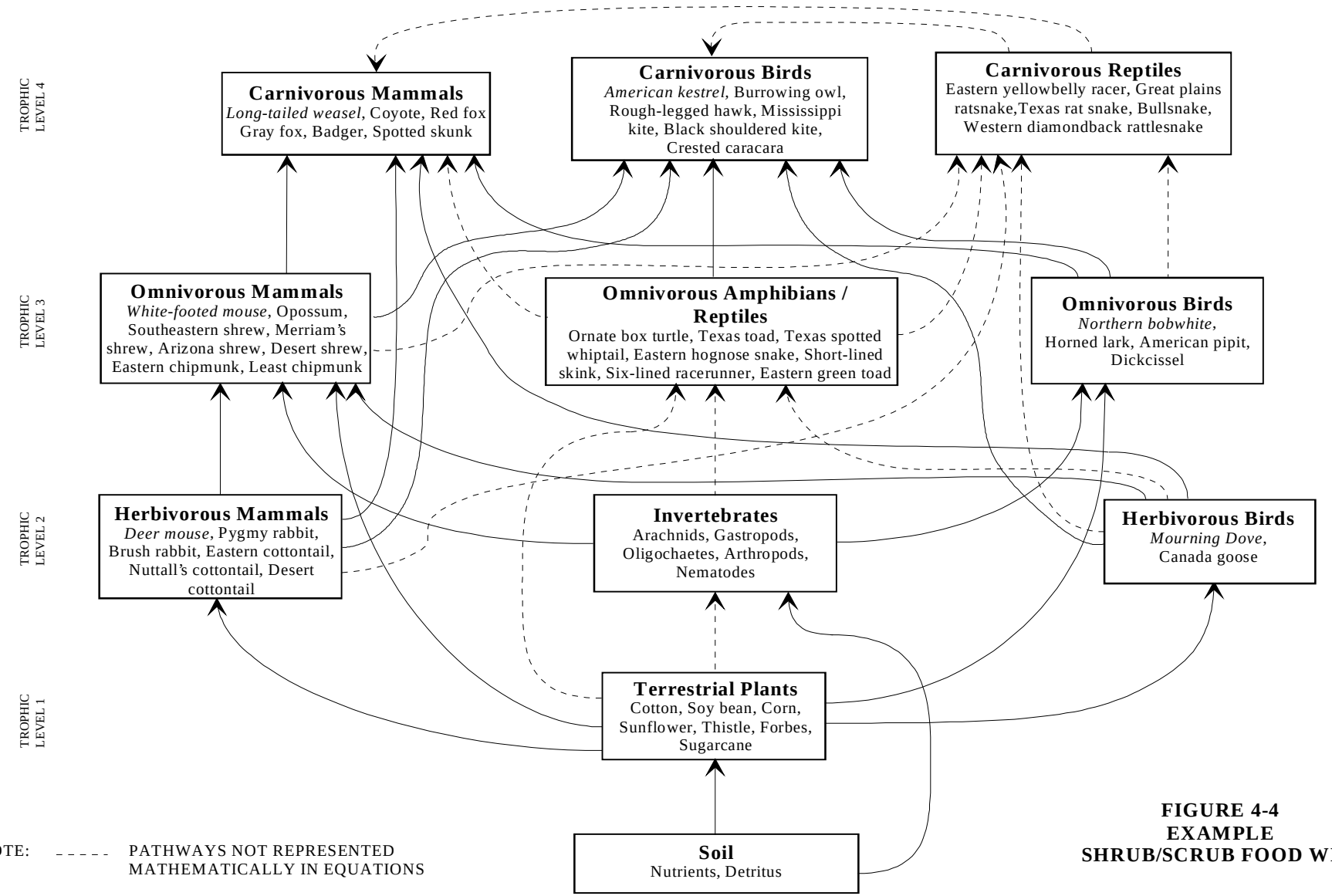


FIGURE 4-4
EXAMPLE
SHRUB/SCRUB FOOD WEB

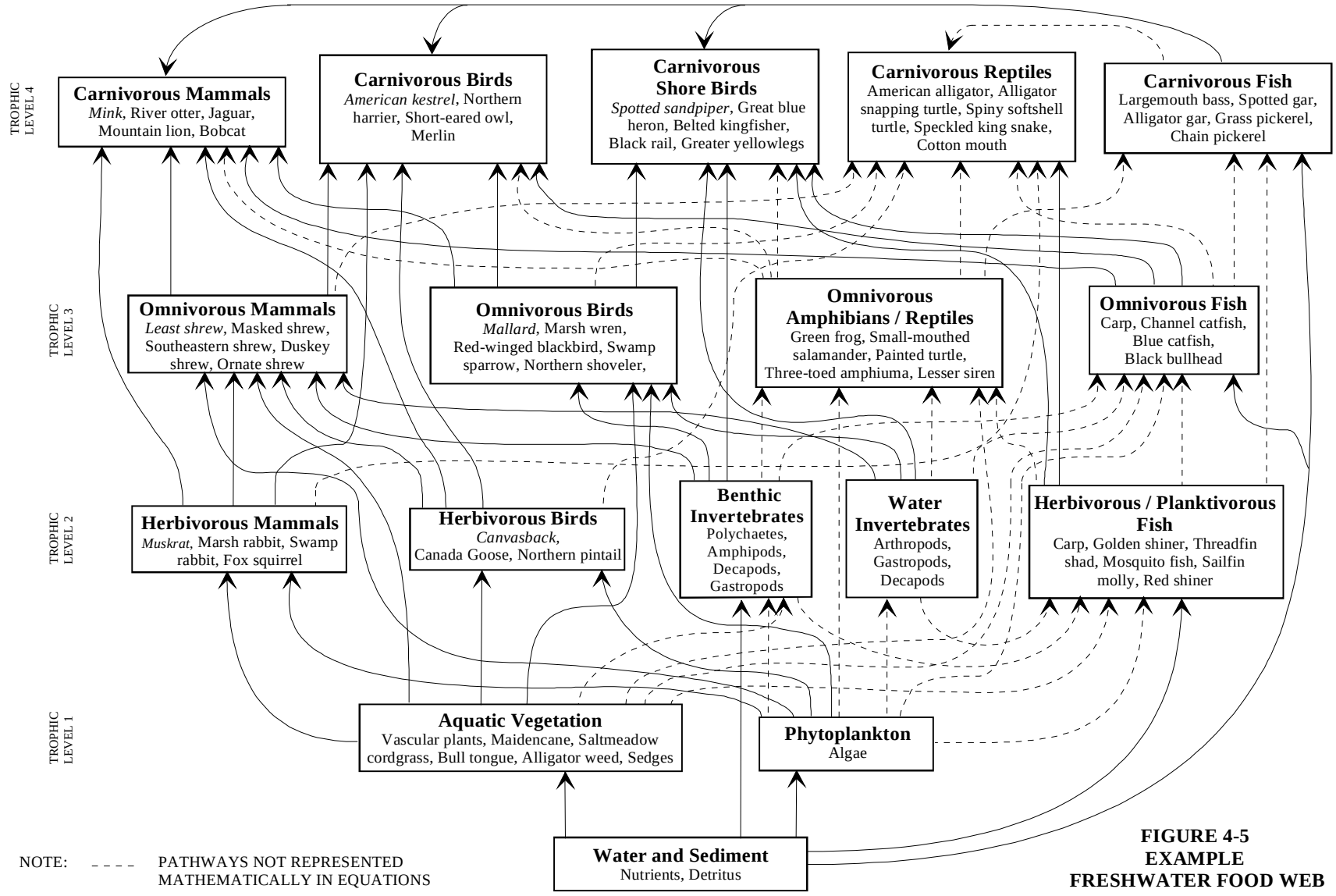


FIGURE 4-5
EXAMPLE
FRESHWATER FOOD WEB

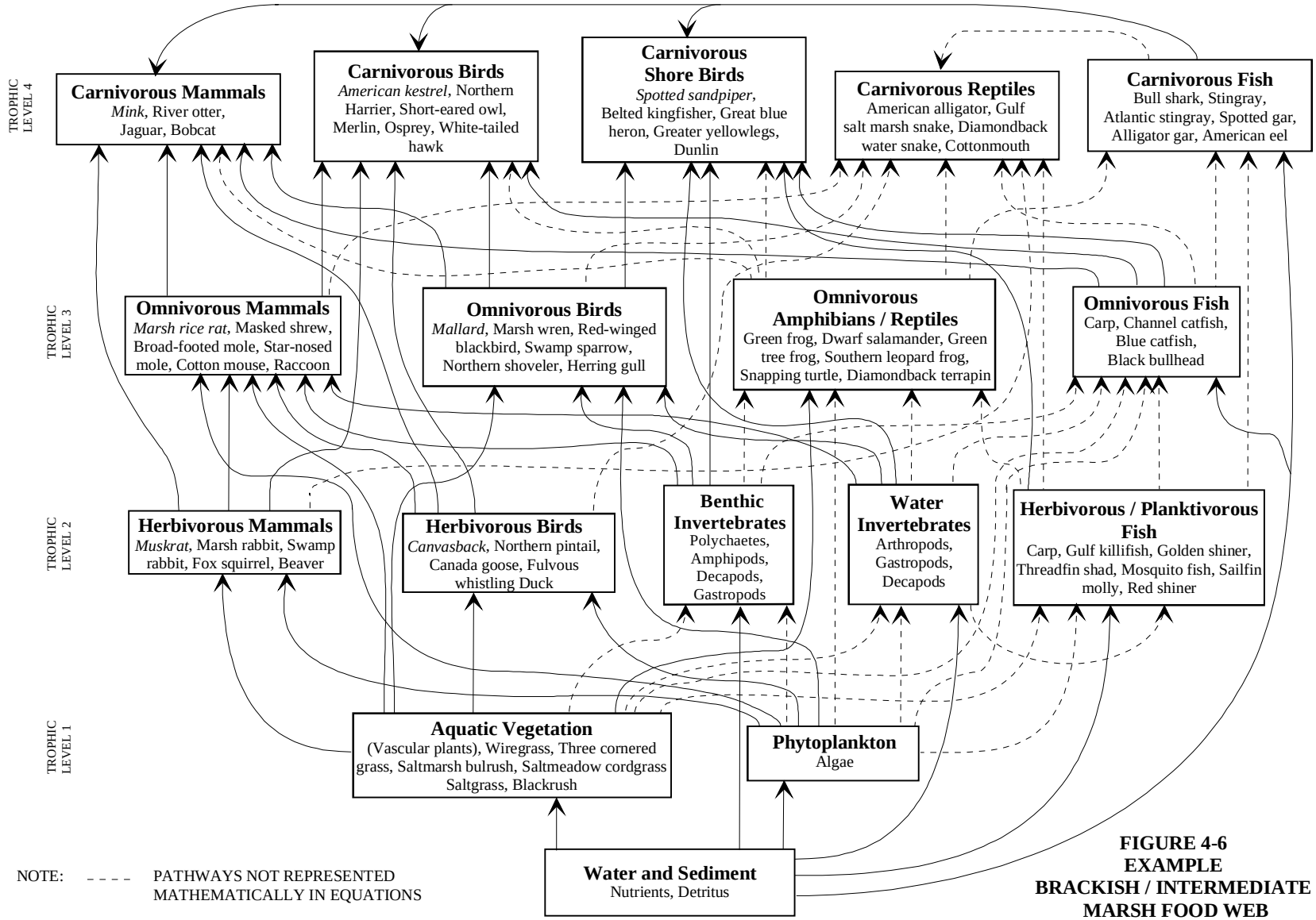


FIGURE 4-6
EXAMPLE
BRACKISH / INTERMEDIATE
MARSH FOOD WEB

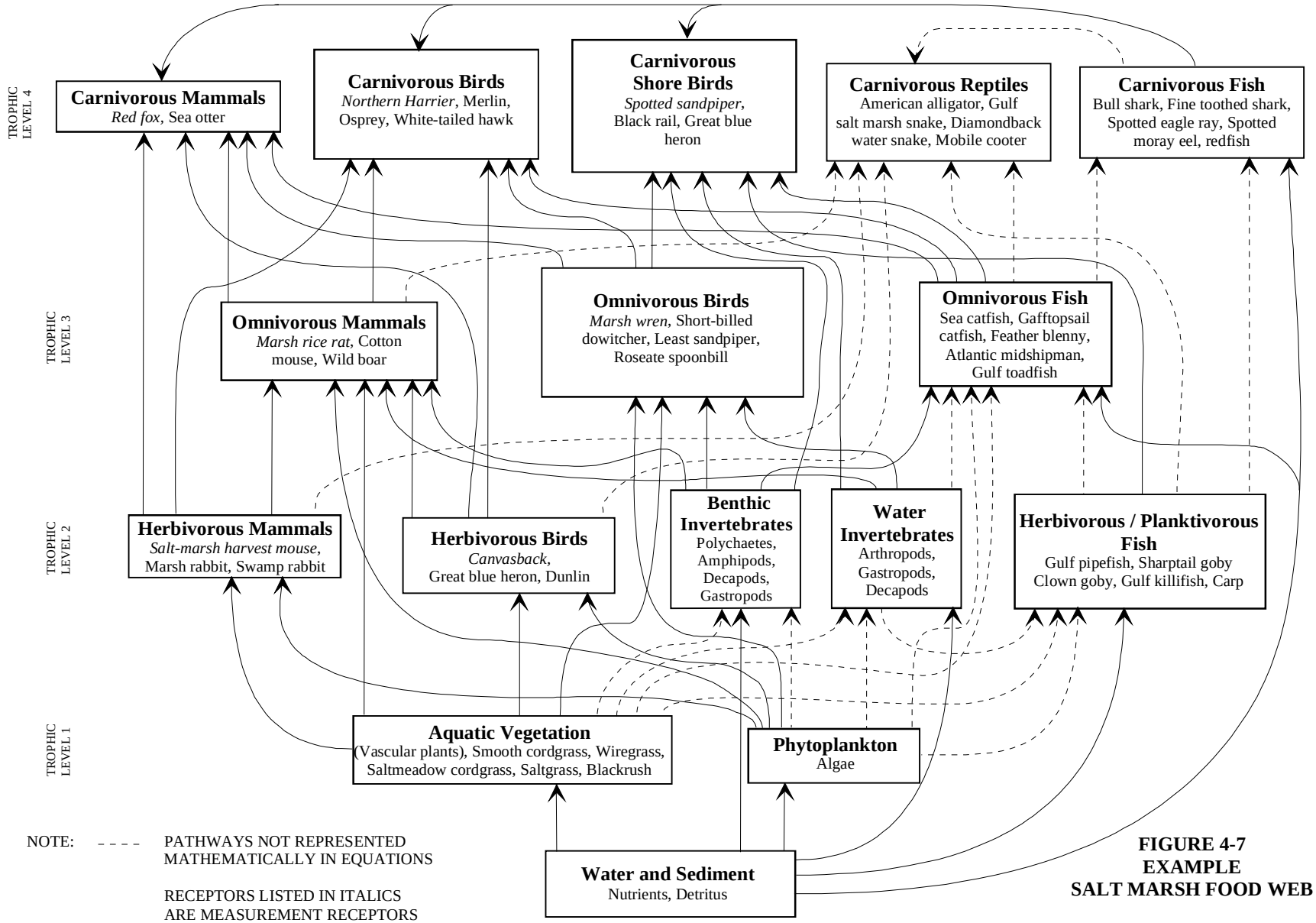


FIGURE 4-7
EXAMPLE
SALT MARSH FOOD WEB

4.3 SELECTING ASSESSMENT ENDPOINTS

An assessment endpoint is an expression of an ecological attribute that is to be protected (U.S. EPA 1997c). A critical ecological attribute of a guild or community is a characteristic that is relevant to ecosystem (food web) structure and function. Protection of the critical ecological attributes of each guild and community is assummed to also ensure the protectiveness of habitat-specific food web structure and function. Therefore, assessment endpoints should be identified specific to each class-specific guild and community within each trophic level of the habitat-specific food web.

Examples of assessment endpoints for guilds include:

- Seed disperser
- Major food source for predator
- Decomposer/detritivore
- Pollinator
- Regulate populations of prey (e.g., forage fish, small rodents)

Examples of assessment endpoints for communities include:

- Diversity or species richness
- Community composition
- Productivity
- Major food source for consumer
- Habitat for wildlife

Descriptions of ecological attributes to be protected (i.e., assessment endpoints) associated with several guilds and communities in a terrestrial ecosystem are provided as examples below.

- Herbaceous plant abundance, habitat, and productivity are attributes to be preserved in a terrestrial ecosystem. As food, herbaceous plants provide an important pathway for energy and nutrient transfer from soil to herbivorous (e.g., rabbit) and omnivorous (e.g., mouse) receptors. Herbaceous plants also provide critically important habitat for small animals.

- Woody plant habitat and productivity are critical attributes to be protected. As food, woody plants provide an important pathway for energy and nutrient transfer from soil to herbivorous and omnivorous vertebrates (e.g., white-tailed deer, yellow-bellied sapsucker). Woody plants also provide critically important habitat for terrestrial wildlife.

- Herbivore productivity is an attribute to be protected in the terrestrial ecosystem because herbivores incorporate energy and nutrients from plants and transfer it to higher trophic levels, such as first- and second-order carnivores (e.g., snakes and owls, respectively). Herbivores also are integral to the success of terrestrial plants, through such attributes as seed dispersal.

- Omnivore productivity is an attribute to be protected in the terrestrial ecosystem because omnivores incorporate energy and nutrients from lower trophic levels and transfer it to higher levels, such as first- and second-order carnivores.

- First-order carnivore productivity is an attribute to be protected in the terrestrial ecosystem because these carnivores provide food to other carnivores (both first- and second-order), omnivores, scavengers, and microbial decomposers. They also affect the abundance, reproduction, and recruitment of lower trophic level receptors, such as vertebrate herbivores and omnivores, through predation.

- Second-order carnivore productivity is an attribute to be protected in the terrestrial ecosystem because carnivores affect the abundance, reproduction, and recruitment of species in lower trophic levels in the food web.

- Soil invertebrate productivity and function as a decomposer are attributes to be preserved in a terrestrial ecosystem, because they provide a mechanism for the physical breakdown of detritus for microbial decomposition, which is a vital function. Soil invertebrates also function as a major food source for omnivorous birds.

Selection of assessment endpoints represents a scientific and management decision point. Since risk characterization, and subsequently final risk management decisions, are dependent on the selection of assessment endpoints, they should be developed with input from risk managers and other stakeholders. Table 4-1 lists the assessment endpoints for guilds and communities in the three aquatic and four terrestrial example habitat-specific food webs.

TABLE 4-1
ASSESSMENT ENDPOINTS FOR GUILDS AND COMMUNITES IN EXAMPLE FOOD WEBS

Representative Receptors		Example Critical Ecological Attributes
Aquatic Receptors		
Aquatic Plants	Phytoplankton, Vascular plants	Primary producers convert light energy into biomass, and are the first link in aquatic food chains supporting higher trophic level aquatic consumers and wildlife. Rooted vegetation also provides habitat and bottom stability.
Water Invertebrates	Crustaceans, Rotifers, Amphipods	Aquatic invertebrates are an important food source for many higher trophic level consumers. Zooplankton regulate phytoplankton populations, and are a critical link in energy transfer to higher trophic levels in aquatic ecosystems.
Herbivorous / Planktivorous Fish	Carp, Gulf killifish, Threadfin shad, Molly, Golden Shiner, Goby, Mosquito Fish, Red Shiner	Herbivorous/Planktivorous Fish are an important prey species for higher trophic level predators in the aquatic and terrestrial ecosystems, and provide a critical link for energy transfer from primary producers to higher trophic level consumers. They generally comprise the majority of tissue biomass in aquatic ecosystems, and provide an important role to the ecosystem through regulating algae and plankton biomass.
Omnivorous Fish	Carp, Channel catfish, Gafftopsail fish, Atlantic midshipman, Feather blenny, Gulf toad fish, Bluecat, Bullhead	Omnivorous fish are an important prey item for higher trophic level predators. Through predation, they may also regulate population levels in lower trophic level fish and invertebrates.
Carnivorous Fish	Largemouth bass, Spotted gar, Bull shark, Redfish, Grass pickerel, Alligator gar, Chain pickerel, American eel, Atlantic stingray, Spotted moray eel, Fine toothed shark	Carnivorous fish provide an important function for the aquatic environment by regulating lower trophic populations through predation. They are also an important prey item for many top level mammal and bird carnivores.
Sediment Receptors		
Sediment Invertebrates	Oligochaetes, Pelecypods, Amphipods, Decapods, Polychaetes, Gastropods	Sediment invertebrates are an important food source for many higher trophic level predators. They also provide an important role as decomposers/detritivores in nutrient cycling.
Soil Receptors		
Terrestrial Plants	Vascular plants, Grasses, Forbs, Lichens	Primary producers provide a critical food source and are the first link in the terrestrial food chain for higher trophic level consumers. In addition, vegetation provides critical habitat for wildlife.

TABLE 4-1 (Continued)
ASSESSMENT ENDPOINTS FOR GUILDS AND COMMUNITES IN EXAMPLE FOOD WEBS

Representative Receptors		Example Critical Ecological Attributes
Soil Invertebrates	Nematodes, Gastropods, Oligochaetes, Arthropods	Soil invertebrates provide an important food source for many higher trophic level species. As decomposers/detritivores they play a critical role in nutrient cycling. They also aid in soil aeration and infiltration by increasing macro, and micro porosity.
Upper Trophic Level Avian and Mammalian Wildlife		
Herbivorous Mammals	Deer mouse, Nutria, Eastern cottontail, Prairie vole, Fox squirrel, Grey squirrel, Swamp rabbit, Eastern wood rat, White-tailed deer, Fulvous harvest mouse, Black-tailed jackrabbit, Hispid cotton rat, Hispid pocket mouse, Black-tailed prairie dog,	Herbivorous mammals are an important prey item for many higher trophic level predators. They provide an important link for energy transfer between primary producers and higher trophic level consumers. In addition, these organisms generally comprise the majority of the terrestrial tissue biomass, and are important in seed dispersal and pollination for many plant species.
Herbivorous Birds	Mourning dove, Canada goose, Chipping sparrow, Northern pintail	Herbivorous birds are an important prey item for many higher trophic level predators. They are important in seed dispersal for many plants in both terrestrial and aquatic ecosystems. Aquatic herbivorous birds may also play an important role in egg dispersion for fish and invertebrate species.
Omnivorous Mammals	Least shrew, Raccoon, Muskrat, Marsh rice rat, Wild boar, Cotton mouse, Eastern spotted skunk, Coyote, Nine-banded armadillo, Virginia opossum, Elliot's short-tailed shrew, Striped skunk, Golden mouse, Seminole bat.	Omnivorous mammals are an important prey item for higher trophic level predators, and influence lower trophic level populations through predation. They play an important role in seed dispersal for many types of terrestrial vegetation and aquatic plants.
Omnivorous Birds	American robin, Northern bobwhite, Marsh wren, Carolina wren, Swamp sparrow, Yellow warbler, Lesser prairie chicken, Roadrunner, Mallard, Least sandpiper, Red cockaded wood pecker, Roseate spoonbill, Greater prairie chicken, Scissor-tailed flycatcher, Sandhill crane, Dickcissel, Canada goose, Red-winged blackbird, Hooded merganser, Northern shovler.	Omnivorous birds are an important prey item for higher trophic level predators. They play an important role in seed dispersal and pollination for many types of terrestrial vegetation and aquatic plants. In addition, aquatic species provide egg dispersal for some fish and invertebrate species.
Omnivorous Amphibians and Reptiles	Ornate box turtle, Green frog, Texas toad, Eastern hognose snake, Plains blind snake, Small-mouthed salamander, Diamondback terrapin, Short-lined skink, Six-lined racerunner, Eastern green toad, Marbled salamander, Slender glass lizard,	Omnivorous amphibians and reptiles provide an important food source for predators. They also provide seed dispersal for many plants and regulate lower trophic level populations through predation.

TABLE 4-1 (Continued)
ASSESSMENT ENDPOINTS FOR GUILDS AND COMMUNITES IN EXAMPLE FOOD WEBS

Representative Receptors		Example Critical Ecological Attributes
Carnivorous Mammals	Grey fox, Swift fox, River otter, Bobcat, Mountain lion, Long-tailed weasel, American badger, Red fox, American mink, Red wolf	Carnivorous mammals provide an important functional role to the environment by regulating lower trophic level prey populations.
Carnivorous Birds	Red-tailed hawk, American kestrel, Marsh hawk, Great-horned owl, Barn owl, Burrowing owl, White-tailed hawk, Ferruginous hawk , Swansons hawk, Golden eagle, Mississippi kite, Prairie hawk, Merlin	Carnivorous Birds provide an important functional role to the environment by regulating lower trophic level prey populations.
Carnivorous Shore Birds	Great blue heron, Belted kingfisher, Spotted sandpiper, Black rail, Greater yellowlegs, Dunlin,	Carnivorous Shore Birds provide an important functional role to the environment by regulating lower trophic level prey populations, and influencing species composition in terrestrial and aquatic ecosystems. They also provide egg dispersal for some fish and aquatic invertebrates.
Carnivorous Reptiles	Eastern yellowbelly racer, Eastern coral snake, Texas rat snake, Western Diamondback rattlesnake, American alligator, Bullsnake, Alligator snapping turtle, Cotton mouth, Speckled king snake, Spiny softshell turtle, Gulf salt marsh snake,	Carnivorous Reptiles provide an important functional role to the environment by regulating lower trophic level prey and are an important prey item for other upper trophic level predators.

4.4 IDENTIFYING MEASUREMENT RECEPTORS TO EVALUATE MEASURES OF EFFECT

Measures of effect are measures used to evaluate "the response of the assessment endpoint when exposed to a stressor (formerly measurement endpoints)" (U.S. EPA 1997c). Measures of exposure are measures of how exposure may be occurring, including how a stressor may co-occur with the assessment endpoint (U.S. EPA 1997c). Measures of effect, in conjunction with measures of exposure, are used to make inferences about potential changes in the assessment endpoint (U.S. EPA 1997c).

Measures of effect are selected as: (1) toxicity values developed and/or adopted by federal or state agencies (e.g., ambient water quality criteria [AWQC], NOAA effects range low [ERL] values) for protection of media-specific communities, or (2) receptor-specific chronic no-observed-adverse-effects-levels (NOAELs) or their equivalent for ecologically relevant endoints (see Chapter 5) for this screening assessment. Measures of exposure are selected as the COPC concentrations in media or dose (e.g., ingestion of contaminated media and/or tissue) to which exposure occurs, and determined as discussed in Chapter 5.

The evaluation of the measure of effect to the assessment endpoint (see Chapters 5 and 6) requires identification of a measurement receptor representive of the assessment endpoint. The measurement receptor is selected based on consideration of factors such as (1) ecological relevance, (2) exposure potential, (3) sensitivity, (4) social or economic importance, and (5) availability of natural history information.

A measurement receptor, specific to each guild, may be selected as a species, population, community, or assemblage of communities. For communities (i.e., soil, surface water, sediment), the community or assemblage of communities is selected as the measurement receptor, and no specific species is selected. For guilds, individual species are selected as measurement receptors. Sections 4.4.1 and 4.4.2 discuss measurement receptors for communities and for mammals and birds, respectively. Section 4.4.3 discusses selection of measurement receptors for the example food webs (see Section 4.2).

4.4.1 Measurement Receptors for Communities

For communities (i.e., soil, surface water, sediment), the community or assemblage of communities are selected as the measurement receptors, and no specific species are selected. Therefore, it is inferred that critical ecological attributes of these communities are not adversely affected if a COPC concentration in that respective media does not exceed the toxicity benchmark specific for that community (see Section 5.1). Representative measurement receptors for soil, surface water, sediment communities include:

- Soil—Soil invertebrate community and terrestrial plant community
- Surface Water—Phytoplankton community, water invertebrate community
- Sediment—Benthic invertebrate community

4.4.2 Measurement Receptor for Guilds

A measurement receptor should be selected for each class-specific guild to model (1) COPC dose ingested, and (2) whole body COPC concentration in prey eaten by predators. The selected measurement receptor should be representative of other species in the guild, with respect to the guild's feeding niche in the ecosystem. The risk assessment should demonstrate that using the measurement receptor ensures that risk to other species in the guild is not underestimated. The following factors should be evaluated to identify a measurement receptor:

- ***Ecological Relevance*** - Highly relevant receptors provide an important functional or structural aspect in the ecosystem. Attributes of highly relevant receptors typically fall under the categories of food, habitat, production, seed dispersal, pollination, and decomposition. Critical attributes include those that affect or determine the function or survival of a population. For example, a sustainable population of forage fish might be critical to the sustainability of a population of carnivorous game fish.
- ***Exposure Potential*** - Receptors with high exposure potentials are those that, due to their metabolism, feeding habits, location, or reproductive strategy, tend to have higher potentials for exposure than other receptors. For example, the metabolic rates of small receptors are generally higher than those for large animals. This results in a higher ingestion per body weight (i.e., increased exposure potential).
- ***Sensitivity*** - Highly susceptible receptors include those with low tolerances to a COPC as well as receptors with enhanced COPC susceptibility due to other concomitant stressors that may not be related to a COPC, such as reduced habitat availability. For example,

raptorial birds are highly sensitive to the effects of chlorinated pesticides that bioaccumulate through the food chain.

- ***Social or Economic Importance*** - An assessment endpoint may also be based on socially or economically important receptors. These types of receptors include species valued for economic importance such as crayfish and game fish. For these receptors, critical attributes include those that affect survival, production, and fecundity characteristics. For example, swamp crayfish are highly sensitive to some heavy metals through adverse effects to behavioral characteristics.

- ***Availability of Natural History Information*** - Natural history information is essential to quantitaviliy evalate risk to measurement receptors. If this information such as body weight, food, water, soil, and sediment ingestion rates is unavailable for the desired measurement receptor, a surrogate species should be selected. Uncertainty associated with using a surrogate species should be discussed.

It should be noted that more than one measurement receptor can be selected per assessment endpoint. Also, although each of these factors should be evaluated when selecting the measurement receptor, at least one of the measurement receptors selected to represent a class-specific guild should have the highest exposure potential (i.e., ingestion rate on a body weight basis). This ensures that risk to other species in the guild is not underestimated.

U.S. EPA's *Wildlife Exposure Factors Handbook* (U.S. EPA 1993o) is an example of an excellent source of dietary and other natural history information. However, it is recommended that receptor information obtained from it or any source be verified and documented during measurement receptor identification.

4.4.3 Measurement Receptors for Example Food Webs

Consistent with the discussions presented in Section 4.4, measurement receptors were selected for the example food webs presented in Section 4.2. Receptor information documented in *Wildlife Exposure Factors Handbook* (U.S. EPA 1993o) and available literature was evaluated to determine suitable measurement receptors for each class-specific guild represented in the example food webs.

Ecological relevance, exposure potential, sensitivity, social or economic importance and availability of natural history information (see Section 4.4.3) were evaluated to identify measurement receptors for the example food webs. It should be noted that since these measurement receptors have been provided as examples to facilitate understanding of the previously described selection process, not every assessment

endpoint has been represented (e.g., TL3 omnivorous fish, TL3 omnivorous amphibians and reptiles, and TL4 carnivorous fish) as may be expected for a complete ecological risk assessment at a site. Discussions on each of the example measurement receptors follow.

American Kestrel

The American kestrel (*Falco sparverius*), or sparrow hawk, was selected as the measurement receptor for the carnivorous bird guild in the example shortgrass prairie, tallgrass prairie, shrub/scrub, freshwater wetland, and brackish/intermediate marsh food webs based on the following information:

- The kestrel is important in regulating small mammal populations through predation. Predators of the kestrel include larger raptors such as red-tailed hawks, golden eagles, and great horned owls.
- The kestrel's prey include a variety of invertebrates such as worms, spiders, scorpions, beetles, and other large insects, as well as an assortment of small to medium-sized birds and mammals. Winter home ranges vary from a few hectares to hundreds of hectares, depending on the amount of available prey in the area.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

American Robin

The American robin (*Turdus migratorius*) was selected as the measurement receptor for the omnivorous bird guild in the example forest food web based on the following information:

- The robin serves an important function in seed dispersion for many fruit species, making it a valuable component of the ecosystem.
- Habitats include forests, wetlands, swamps, and habitat edge where forested areas are broken with agricultural and range land. The robin forages on snails and other soil invertebrates, seeds, and fruit.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Canvasback

The Canvasback (*Aythya valisineria*) was selected as the measurement receptor for the herbivorous bird guild in all three example aquatic food webs based on the following information:

- The Canvasback provides a valuable functional role to aquatic habitats by dispersing seeds for aquatic vegetation.
- The Canvasback is the largest member of the Pochards (bay ducks) and is common throughout North America. They breed from Alaska to Nebraska, and in intermountain marshes of Washington, Oregon, and northern California. Their diet consists of aquatic vegetation, and small invertebrates, which they obtain by digging in sediments. Although the canvasback consumes aquatic invertebrates during certain times of the year, in winter when they are present along coastal regions, a large portion of their diet is aquatic vegetation and was therefore selected to represent the herbivorous bird guild.
- Since natural history information on the canvasback was scarce, the Lesser Scaup (*Aythya affinis*), for which natural history information is readily available, was selected as a surrogate receptor.

Deer Mouse

The deer mouse (*Peromyscus maniculatus*) was selected as the measurement receptor for the herbivorous mammal guild in the example forest, shortgrass prairie, tallgrass prairie, shrub/scrub food webs based on the following information:

- The deer mouse is preyed upon by owls, snakes, and small carnivorous mammals, making it a very important prey item. This animal also plays an important ecological role in seed and fruit dispersion for many types of vegetation. In addition, their burrowing activities influence soil composition and aeration.
- The deer mouse is almost strictly nocturnal and feeds chiefly on seeds, fruits, bark, roots, and herbage. Due to its burrowing and dietary habits, there is a high potential for direct and indirect exposure. The home range for a deer mouse is rarely over 100 meters, and it spends most of its day in an underground burrow.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Least Shrew

The least shrew (*Cryptotis parva*) was selected as the measurement receptor for the omnivorous mammal guild in the example tallgrass prairie, shortgrass prairie, and freshwater wetland food webs based on the following information:

- Because of the shrews abundance and high population density, they make up a large portion of the diet of owls, hawks, and snakes.
- Shrews feed on snails, insects, sow bugs, and other small invertebrates. The home range size is on average 0.39 hectares. Their diet of invertebrates and their burrowing behavior result in a high potential of direct and indirect exposure to contaminants.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Long-tailed Weasel

The long-tailed weasel (*Mistily Renata*) was selected as the measurement receptor for the carnivorous mammal guild in the example forest, tallgrass prairie and shrub/scrub food webs based on the following information:

- The long-tailed weasel is important in regulating small mammal populations through predation. Predators of the weasel include cats, foxes, snakes, and large raptors such as hawks and owls.
- Habitats are varied and include forested, brushy, open areas including farm lands preferably near water, where they prey on rabbits, chipmunks, shrews, mice, rats and birds.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Mallard Duck

The mallard duck (*Anas platyrhynchos*) was chosen as the measurement receptor for the omnivorous bird guild for the freshwater wetland and brackish/intermediate marsh food webs based on the following information:

- The mallard serves as a valuable component in aquatic food webs providing dispersion of seeds for aquatic vegetation, and due to their role in the nutrient cycle of wetlands. In addition, the mallard is a major prey item for carnivorous mammals, birds, and snakes.

- The mallard is present in a diverse amount of aquatic habitats throughout the United States. Although their diet is considered omnivorous, 90 percent of their diet may be plant material at some times of the year. Mallards are surface feeders that will often filter through soft mud and sediment searching for food items.

- The mallard is very important game species, representing approximately one-third of all waterfowl harvested.

- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Marsh Rice Rat

The marsh rice rat (*Oryzomys palustris*) was selected as the measurement receptor for the omnivorous mammal guild in the example brackish/intermediate and salt marsh food web based on the following information:

- The marsh rice rat inhabits marsh and wetland areas where it feeds on crabs, insects, fruits, snails, and aquatic plants. The rice rat plays an important role in seed dispersal and is a major food item for many predators including raptors, cats, weasels and snakes.

- The marsh rice rat has a high potential for exposure due to their aquatic diet and direct contact with media.

- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Marsh Wren

The marsh wren (*Cistothorus palustris*) was selected as the measurement receptor for the omnivorous bird guild in the example salt marsh food web based on the following information:

- The marsh wren consumes large numbers of aquatic insects thus regulating their populations, which make it a valuable component of the ecosystem. Main predators are snakes and turtles which prey heavily upon the eggs.

- The marsh wren is common throughout the United States, inhabiting freshwater, brackish, and saltwater marshes. Its diet consists mainly of aquatic invertebrates, although snails

and spiders may be taken. In addition, its diet of aquatic invertebrates makes it susceptible to accumulation and toxicity of bioaccumulative chemicals

- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Mink

The mink (*Mustela vison*) was selected as the measurement receptor for the carnivorous mammal guild in the example brackish/intermediate marsh and freshwater food webs based on the following information:

- As a high trophic level predator, the mink provides an important component to the ecosystem by influencing the population dynamics of their prey. Their main predators include fox, bobcats, and great-horned owls.

- The mink is one of the most abundant carnivorous mammals in North America, inhabiting rivers, creeks, lakes, and marshes. They are distributed throughout North America, except in extreme north Canada, Mexico, and areas of the southwestern United States. Mink are predominantly nocturnal hunters, although they are sometimes active during the day. They are opportunistic feeders and will consume whatever prey is most abundant including: small mammals, fish, birds, reptiles, amphibians, crustaceans, and insects.

- They have been shown to be sensitive to PCBs and similar chemicals, and have a high potential for exposure due to their aquatic diet and direct contact with the media.

- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Mourning Dove

The Mourning Dove (*Zenaida macroura*) was selected as the measurement receptor for the herbivorous bird guild in all four example terrestrial food webs based on the following information:

- The dove plays an important functional role in seed dispersion for many grasses and forbs. Doves provide an important prey item for many higher trophic level omnivores and carnivores. Predators of the mourning dove include falcons, hawks, fox, and snakes.

- The mourning dove inhabits open woodlands, forests, prairies, and croplands. It feeds mostly on seeds, which comprise 99 percent of its diet. It may ingest insignificant amounts of animal matter and green forage incidently.

- Mourning doves have a high potential for exposure through ingestion of inorganic contaminants.

- Mourning doves are an important game species, contributing significantly as a food and economic resource.

- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Muskrat

The muskrat (*Ondrata zibethicus*) was selected as the measurement receptor for the herbivorous mammal guild in the example freshwater wetland and brackish/intermediate marsh food webs based on the following information:

- The muskrat is important to the overall structure of the aquatic ecosystem by regulating aquatic vegetation diversity and biomass, resulting in stream bank stability and increased habitat diversity for aquatic organisms including fish. It was also chosen as the measurement receptor based on its value to the ecosystem including its large population densities and importance as a prey species (e.g., prey for hawks, mink, otters, owls, red fox, snapping turtles, alligators, and water snakes).

- The muskrat spends a large part of its time in the water, and is common in fresh, brackish, and saltwater habitats. It has relatively high food and water ingestion rates, and a diet that consists mainly of aquatic vegetation, clams, crayfish, frogs, and small fish.

- Due to the large numbers, the muskrat plays an important economic role in the fur industry, and as a food item for some cultures.

- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Northern Bobwhite

The northern bobwhite (*Colinus virginianus*) was selected as the measurement receptor for the omnivorous bird guild in the example shortgrass prairie and shrub/scrub food webs based on the following information:

- The bobwhite plays an important role in seed dispersion for many plant species, and is an important prey item for snakes, and other small mammals. If habitat conditions permit, their numbers will increase rapidly, providing an additional food source for many predators. They also are valuable in controlling insect populations during certain times of the year.

- The bobwhite's diet consists mainly of seeds and invertebrates, although in the winter green vegetation can dominate its diet. During breeding season, the bobwhite's home

range may encompasses several hectares, including areas for foraging, cover, and a nest site. In non-breeding season, the bobwhite's home range can be as large as 16 hectares. It has a high potential for exposure through ingestion and dermal contact with soil during dust bathing.

- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Northern Harrier

The Northern harrier (*Circus cyaneus*), also called the Marsh hawk was selected as the measurement receptor for carnivorous bird guild in the example salt marsh food web based on the following information:

- The marsh hawk plays an important role in the ecosystem in regulating small mammal populations through predation.
- The marsh hawks diet consists of small mammals, birds, and occasionally snakes, frogs, and insects. Their habitat preferences include wetlands or marshes.
- In addition, the marsh hawk has demonstrated sensitivity to pesticides, which bioaccumulate through food chains.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Red Fox

The red fox (*Vulpes vulpes)* was selected as the measurement receptor for the carnivorous mammal guild in the example salt marsh food web based on the following information:

- Red fox have a high potential for exposure due to bioaccumulation though the food chain, and are a valuable component to ecosystem structure by regulating the abundance, reproduction, distribution, and recruitment of lower trophic level prey.
- Although omnivorous in dietary habits, the majority of the diet consists of cottontail rabbits, voles, mice, birds, and other small mammals. This animal was chosen because of its status as a top carnivore and its widespread distribution in the United States, inhabiting chaparral, wooded and brushy areas, coastal areas and rim rock country.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Red-tailed Hawk

The red-tailed hawk (*Buteo jamaicensis*) was selected as the measurement receptor in the carnivorous bird guild in the example forest food web based on the following information:

- The red-tailed hawks position as a high trophic level predator makes them a valuable component of terrestrial food webs through their regulation of populations of lower trophic level prey species.
- The red-tailed hawk is widely distributed in the United States among a diverse number of habitat types ranging from woodlands to pastures. Its diet includes small mammals (such as mice, shrews, voles, rabbits, and squirrels), birds, lizards, snakes, and large insects. It is an opportunistic feeder, preying on whatever species is most abundant. Red-tailed hawks are territorial throughout the year, and have home ranges that can be over 1,500 hectares.
- Red-tailed hawks have shown sensitivity to many chemicals which disrupt reproduction or egg development.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Salt Marsh Harvest Mouse

The salt marsh harvest mouse (*Reithrodontomys raviventris*) was selected as the measurement receptor for the herbivorous mammal guild in the example salt marsh food web based on the following information:

- The salt marsh harvest mouse plays an important functional role in aquatic habitats through seed dispersal for aquatic vegetation.
- Predators include owls, snakes, and many mammals including weasels, fox, and cats.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Short-tailed Shrew

The short-tailed shrew (*Blarina brevicauda*) was selected as the measurement receptor for the omnivorous mammal guild in the example forest food web based on the following information:

- The short-tailed shrews value as a prey species for many high level predators is very important to the health of an ecosystem. They also play an important role in soil recycling and aeration, through tunnel excavation.

- The short-tailed shrew is one of the most common mammals in the United States. It is a small insectivorous mammal that represents secondary consumers (insectivores) present in terrestrial ecosystems. Their diet of invertebrates such as earthworms and their burrowing behavior result in a high potential of direct and indirect exposure to contaminants It has a very high metabolism rate which requires almost constant feeding. The most common habitats are wooded and wet areas in the drier parts of the range.

- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Spotted Sandpiper

The spotted sandpiper (*Actitis macularia*) was selected as the measurement receptor for the carnivorous shore bird guild in the example freshwater wetland, brackish/intermediate, and salt marsh food webs based on the following information:

- The spotted sandpiper inhabits a wide variety of habits usually associated with water or marsh.

- Spotted sandpipers have a high potential for exposure through ingestion of aquatic insects, worms, fish , crustaceans, mollusks, and carrion.

- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Swift Fox

The Swift Fox (*Vulpes velox*) was selected as the measurement receptor for the carnivorous mammal guild in the example shortgrass prairie food web based on the following information:

- The swift fox fills an important functional role by regulating the population dynamics of many prey species.

- The swift fox is mainly nocturnal and its diet consists of small mammals, insects, birds, lizards, and amphibians. It spends most of its days in a den, emerging at night to hunt. Their home range extends several kilometers.

- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Western Meadow Lark

The western meadow lark (*Sturnella neglecta*) was selected as the measurement receptor for the omnivorous bird guild in the example tallgrass prairie food web based on the following information:

- The western meadow lark serves an important function in seed dispersion for many forb and grass species, making it a valuable component of the ecosystem.
- Habitats include grassland, savanna, pasture, and cultivated fields. The western meadow lark forages on spiders, sowbugs, snails, and grass and forb seeds.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

White-footed Mouse

The white-footed mouse (*Peromyscus polionotus*) was selected as the measurement receptor for the omnivorous mammal guild in the example shrub/scrub food web based on the following information:

- The white-footed mouse plays an important role in seed dispersal and provide an important food source for raptors, snakes and other mammals including cats, weasels and fox.
- The white-footed mouse feeds on nuts, seeds, fruits, beetles, caterpillars, and other insects. Due to its burrowing and dietary habits, there is a high potential for direct and indirect exposure.
- The availability of natural history information (e.g., home range, ingestion rates, body weights) also support selection as a measurement receptor.

Chapter 5
Analysis

What's Covered in Chapter 5:

- Exposure Assessment
- Toxicity Assessment

The analysis phase of a risk assessment consists of assessing (1) exposure of a measurement receptor to a compound of potential concern (COPC), and (2) toxicity of a COPC to a measurement receptor. The exposure assessment (Section 5.1), and the toxicity assessment (Section 5.4) are used to characterize ecological risk, as discussed in Chapter 6.

5.1 EXPOSURE ASSESSMENT

Exposure is the contact (e.g., ingestion) of a receptor with a COPC. Exposure of ecological receptors to COPCs emitted from facility sources are evaluated through consideration of exposure pathways. All exposure pathways that are potentially complete should be evaluated. The existence of a potentially complete exposure pathway indicates the potential for a receptor to contact a COPC; it does not require that a receptor be adversely affected. Exposure pathways considered in this guidance include all direct uptake pathways of a COPC from media (e.g., soil, sediment, and surface water) for lower trophic level receptors evaluated at the community level, and ingestion of a COPC contaminated organism (plant or animal food item) or media for higher trophic level receptors evaluated as class-specific guilds. It should be noted that exposure pathways currently not addressed in this guidance due to the limitation of data include (1) inhalation and dermal exposure pathways for upper trophic level organisms, (2) ingestion via grooming and preening, and (3) foliar uptake of dissolved COPCs by aquatic plants.

Exposure assessment consists of quantifying exposure of a measurement receptor to a COPC. As previously noted (see Chapter 4), exposure to community and class-specific guild measurement receptors is assessed using different approaches. This is because the available toxicity reference values (*TRV*s) used in

risk characterization (see Chapter 6) for lower trophic level communities are media specific; whereas *TRV*s for upper trophic level class-specific guilds are provided in terms of dose ingested.

For community measurement receptors (e.g., water, sediment, and soil communities), the exposure assessment consists of determining the COPC concentration in the media that the particular community inhabits. For example, the COPC concentration in soil is determined during the exposure assessment for comparison to the NOAEL for terrestrial plants and soil invertebrates during risk characterization. For class-specific guild measurement receptors, exposure is assessed by quantifying the daily dose ingested of contaminated media and/or organism (expressed as the mass of COPC ingested per kilogram body weight per day). The following sections provide guidance on assessing exposure to community and class-specific guild measurement receptors.

5.2 Assessing Exposure to Community Measurement Receptors

Since exposure to communities is assumed to be primarily through contact with COPCs within the media they inhabit, the assessment of exposure for community measurement receptors is simply the determination of the COPC concentration in the media that they inhabit. Exposure for water, sediment, and soil community measurement receptors should be determined as follows:

> ***Water Community*** **-** Exposure to the water community as a measurement receptor (e.g., water invertebrates or phytoplankton in the freshwater/wetland food web) is assessed by determining the COPC dissolved water concentration (*Cdw*) (see Chapter 3 and Appendix B) at the specific location being evaluated (see Chapter 4).
>
> ***Sediment Community*** **-** Exposure to the sediment community as a measurement receptor (e.g., sediment invertebrates in the brackish/intermediate food web) is assessed by determining the COPC concentration in bed sediment (*Csed*) (see Chapter 3 and Appendix B) at the specific location being evaluated (see Chapter 4).
>
> ***Soil Community*** **-** Exposure to the soil community as a measurement receptor (e.g., soil invertebrates or terrestrial plants in the forest food web) is assessed by determining the COPC concentration in soil (*Cs*) (see Chapter 3 and Appendix B) at the specific location being evaluated (see Chapter 4).

5.3 Assessing Exposure to Class-Specific Guild Measurement Receptors

Exposure to measurement receptors of class-specific guilds is assessed by quantifying the daily dose ingested of contaminated food items (i.e., plant and animal), and media. COPC daily dose ingested (expressed as the mass of COPC ingested per kilogram body weight per day) depends on the COPC concentration in plant and animal food items and media, the measurement receptor's trophic level (i.e., consumer), the trophic level of animal food items (i.e., prey), and the measurement receptor's ingestion rate of each food item and media. The complexity of the daily dose equation will depend on (1) the number of food items in a measurement receptor's diet, (2) the trophic level of each food item and of the measurement receptor. The daily dose of COPC ingested by a measurement receptor, considering all food items and media ingested, can be calculated from the following generic equation:

$$DD = \sum IR_F \cdot C_i \cdot P_i \cdot F_i + \sum IR_M \cdot C_M \cdot P_M \qquad \text{Equation 5-1}$$

where

DD	=	Daily dose of COPC ingested (mg COPC/kg BW-day)
IR_F	=	Measurement receptor plant or animal food item ingestion rate (kg/kg BW-day)
C_i	=	COPC concentration in *i*th plant or animal food item (mg COPC/kg)
P_i	=	Proportion of *i*th food item that is contaminated (unitless)
F_i	=	Fraction of diet consisting of plant or animal food item *i* (unitless)
IR_M	=	Measurement receptor media ingestion rate (kg/kg BW-day [soil or bed sediment] or L/kg BW-day [water])
C_M	=	COPC concentration in media (mg/kg [soil or bed sediment] or mg/L [water])
P_M	=	Proportion of ingested media that is contaminated (unitless)

Sections 5.3.1 through 5.3.2 (also see Appendix F) provide guidance for determining values for the above parameters; including (1) the determination of measurement receptor food item and media ingestion rates, and (2) the calculation of COPC concentrations in plant and animal food items. The use of *BCF*s and *FCM*s in calculating COPC concentrations in plant and animal food items is also discussed in the following sections. The daily dose should be computed using COPC media (i.e., soil, sediment, surface water, air) concentrations, at the location within the habitat supporting the food web being evaluated (see Chapter 4), for determination of (1) the COPC concentration in the plant or animal food item ingested, and (2) the

COPC concentration in the media ingested. Guidance on the calculation of COPC concentrations in media being ingested is provided in Chapter 3 and Appendix B.

The daily dose of COPC ingested by a measurement receptor should be determined by summing the contributions from each contaminated plant, animal, and media food item. Equation 5-1 and consumer specific equations in Appendix F, are derived to account for 100 percent of the measurement receptor's diet (total daily mass of food items ingested) which can potentially be contaminated. However, if a food item or media at an actual site location is not contaminated (i.e., the COPC concentration in the media or resulting food item is zero), then the daily mass of that food item or media ingested does not contribute to the daily dose of COPC ingested. Also, Equation 5-1 does not directly include a term for home range, as defined spatially. However, the term accounting for the proportion of plant or animal food item that is contaminated, P_i, numerically accounts for the fraction of a respective food item that may potentially be obtained from outside the geographical limits of the impacted habitat (i.e., outside the area of contamination) being evaluated.

For measurement receptors ingesting more than one plant or animal food item, U.S. EPA OSW recommends that exposure be separately quantified assuming that the measurement receptor ingests both "equal" and "exclusive" diets. Not only does this constitute the most complete evaluation of exposure potential for a measurement receptor; if warranted, it also identifies which pathways are driving risk specific to a COPC and measurement receptor, and allows risk management efforts to be prioritized. Guidance for calculating *DD* assuming "equal diet" and "exclusive diet" is provided below.

> ***Equal Diet*** - To evaluate exposure to a measurement receptor based on an equal diet, the daily dose of COPC ingested is calculated assuming that the fraction of daily diet consumed by the measurement receptor is equal among food item groups. This is computed by setting the value for fraction of diet consisting of plant and/or animal food items, F_i, equal to 1.0 divided by the total number of plant and animal food item groups ingested. Therefore, F_i values within a specific *DD* equation would be the same numerically.
>
> ***Exclusive Diet*** - To evaluate exposure to a measurement receptor based on exclusive diets, the daily dose of COPC ingested is calculated assuming that the fraction of daily diet consumed by the measurement receptor is exclusively (100 percent) one food item group. This is computed by setting the value for F_i equal to 1.0 for each food item group at a time, while the F_i values for the remaining food item groups are set equal to zero. The food item designated as exclusive is alternated to each respective food item represented in the *DD* equation to obtain a numeric range of exposure values based on exclusive diets. If the daily diet of a food item (i.e., prey) of a measurement receptor (i.e., consumer) also consists of more than one plant or animal food item,

then an equal diet should be assumed for the food item being consumed while evaluating exposure to the measurement receptor.

In addition to quantifying exposure based on equal and exclusive diets for measurement receptors, U.S. EPA OSW recommends that the following assumptions be applied in a screening level risk assessment.

- The COPC concentrations estimated to be in food items and media ingested are bioavailabile.
- Only contributions of COPCs from the sources (e.g., combustion stacks, fugitives) included in the risk assessment are considered in estimating COPC concentrations in food items and media.
- The measurement receptor's most sensitive life stage is present in the assessment area being evaluated in the risk assessment.
- The body weights and food ingestion rates for measurement receptors are conservative.
- Each individual species in a community or class-specific guild is equally exposed.
- The proportion of ingested food items and ingested media that is contaminated is assumed to be 100 percent (i.e., P_i is asigned a value of 1.0); which assumes that a measurement receptor feeds only in the assessment area.

Although conservative in nature, U.S. EPA OSW recommends use of these assumptions considering that the results of a screening level risk assessment are intended to support development of permits and focus risk management efforts. Site-specific exposure characterization that my warrant deviation from these screening level assumptions should be reviewed and approved by the appropriate permitting authority following recommendations provided in Section 3.12.

5.3.1 Ingestion Rates for Measurement Receptors

As indicated in Equation 5-1 above, species specific ingestion rates of food items and media, on a body weight basis, are required for calculating the daily dose of COPC ingested for each measurement receptor. As specified for use in the equations presented in Appendix F, it is important to ensure that food (i.e., plants and animals) and water ingestion rates are on a wet weight basis, and ingestion rates for soil and sediment are on a dry weight basis (see Appendix F). Table 5-1 provides values for ingestion rates for measurement receptors identified in the example food webs presented in Chapter 4. These values are primarily obtained from the allometric equations presented in the *Wildlife Exposure Factors Handbook*

(U.S. EPA 1993o). Soil ingestion rates were calculated using the percent soil in estimated diets of wildlife as described in Beyer et al. (1994).

Species specific ingestion rates including food and water have been measured for few wildlife species. Therefore, allometric equations presented in the *Wildlife Exposure Factors Handbook* were used to calculate species specific food and media ingestion rates. Allometry is defined as the study of the relationship between the growth and size of one body part to the growth and size of the whole organism, including ingestion rates, and can be used to estimate species specific values for ingestion (U.S. EPA 1993o). Allometric equations should only be used for those taxonomic groups used to develop the allometric relationship. For example, equations developed for carnivorous mammals should not be used to calculate food ingestion rates for herbivorous mammals. For a detailed discussion on the development and limitations of the allometric equations used to obtain ingestion rate values presented in Table 5-1, see U.S. EPA (1993o) and Nagy (1987).

The use of individual species body weights may result in some uncertainty, since individual species usually exhibit values somewhat different from those predicted by allometric modeling derived using multiple species. However, this uncertainty is expected to be minimal since measurement receptors were selected to maximize exposure for each class-specific guild, as discussed in Section 4.4.2.

If species specific values are not available in U.S. EPA (1993o), or can not be represented by the allometric equations presented, other sources to evaluate include:

- U.S. Fish and Wildlife Service (FWS) publications (e.g., U.S. FWS 1979)
- State wildlife resource management agencies
- Published scientific literature
- Publications by wildlife conservation organizations (such as The National Audubon Society)

TABLE 5-1

INGESTION RATES FOR EXAMPLE MEASUREMENT RECEPTORS

Measurement Receptor	Example Food Web[a]	Body Weight (kg)	Reference	Food IR [e] (kg WW/ kg BW-day)	Reference	Water IR (L /kg BW-day)	Reference	Soil/Sed IR [m] (kg DW/ kg BW-day)	Reference
American Kestrel	SG, TG, SS, FW, BR	1.00E-01	U.S. EPA 1993o	4.02E-01 [f]	U.S. EPA 1993o; Nagy 1987	1.25E-01 [k]	U.S. EPA 1993o	1.39E-03 [n]	Pascoe et al. 1996
American Robin	F	8.00E-02	U.S. EPA 1993o	4.44E-01 [f]	U.S. EPA 1993o; Nagy 1987	1.37E-01 [k]	U.S. EPA 1993o	1.43E-02 [o]	Beyer et al. 1994
Canvas Back	FW, BR, SW	7.70E-01 [b]	U.S. EPA 1993o	1.99E-01 [f]	U.S. EPA 1993o; Nagy 1987	6.43E-02 [k]	U.S. EPA 1993o	1.82E-03 [p]	Beyer et al. 1994
Deer Mouse	TG, F, SG, SS	1.48E-02	U.S. EPA 1993o	5.99E-01 [g]	U.S. EPA 1993o; Nagy 1987	1.51E-01 [l]	U.S. EPA 1993o	1.44E-03 [q]	Beyer et al. 1994
Least Shrew	SG, FW, TG	4.00E-03	National Audubon Society 1995	6.20E-01 [h]	U.S. EPA 1993o	1.72E-01 [l]	U.S. EPA 1993o	1.36E-02 [o]	Beyer et al. 1994
Long Tailed Weasel	TG ,F, SS	8.50E-02	National Audubon Society 1995	3.33E-01 [i]	U.S. EPA 1993o; Nagy 1987	1.27E-01 [l]	U.S. EPA 1993o	2.98E-03 [r]	Beyer et al. 1994
Mallard Duck	BR, FW	1.04E+00	U.S. EPA 1993o	1.79E-01 [f]	U.S. EPA 1993o; Nagy 1987	5.82E-02 [k]	U.S. EPA 1993o	3.18E-03	Beyer et al. 1994
Marsh Rice Rat	BR, SW	3.00E-02	National Audubon Society 1995	4.40E-01 [g]	U.S. EPA 1993o; Nagy 1987	1.41E-01 [l]	U.S. EPA 1993o	2.33E-03 [s]	Beyer et al. 1994
Marsh Wren	SW	1.00E-02	U.S. EPA 1993o	9.26E-01 [f]	U.S. EPA 1993o; Nagy 1987	2.75E-01 [k]	U.S. EPA 1993o	1.96E-02 [o]	Beyer et al. 1994
Mink	FW, BR	9.74E-01	U.S. EPA 1993o	2.16E-01 [i]	U.S. EPA 1993o; Nagy 1987	9.93E-02 [l]	U.S. EPA 1993o	1.93E-03 [r]	Beyer et al. 1994

TABLE 5-1

INGESTION RATES FOR EXAMPLE MEASUREMENT RECEPTORS

Measurement Receptor	Example Food Web[a]	Body Weight (kg)	Reference	Food IR [e] (kg WW/ kg BW-day)	Reference	Water IR (L /kg BW-day)	Reference	Soil/Sed IR [m] (kg DW/ kg BW-day)	Reference
Mourning Dove	F, SS, TG, SG	1.50E-01 [c]	U.S. EPA 1993o	3.49E-01 [f]	U.S. EPA 1993o; Nagy 1987	1.09E-01 [k]	U.S. EPA 1993o	7.01E-03 [o]	Beyer et al. 1994
Muskrat	BR, FW	1.09E+00	U.S. EPA 1993o	2.67E-01 [j]	U.S. EPA 1993o; Nagy 1987	9.82E-02 [l]	U.S. EPA 1993o	6.41E-04	Beyer et al. 1994
Northern Bobwhite	SG, SS	1.50E-01	U.S. EPA 1993o	3.49E-01 [f]	U.S. EPA 1993o; Nagy 1987	1.09E-01 [k]	U.S. EPA 1993o	1.20E-02 [t]	Beyer et al. 1994
Northern Harrier	SW	9.60E-01	U.S. EPA 1993o	1.85E-01 [f]	U.S. EPA 1993o; Nagy 1987	5.99E-02 [k]	U.S. EPA 1993o	9.95E-03 [n]	Beyer et al. 1994
Red Fox	SW	3.94E+00	U.S. EPA 1993o	1.68E-01 [i]	U.S. EPA 1993o; Nagy 1987	8.63E-02 [l]	U.S. EPA 1993o	1.51E-03	Beyer et al. 1994
Red-tailed Hawk	F	9.60E-01 [d]	U.S. EPA 1993o	1.85E-01 [f]	U.S. EPA 1993o; Nagy 1987	5.99E-02 [k]	U.S. EPA 1993o	9.95E-03 [n]	Beyer et al. 1994
Salt-marsh Harvest Mouse	SW	9.10E-03	U.S. EPA 1993o	7.41E-01 [g]	U.S. EPA 1993o; Nagy 1987	1.58E-01 [l]	U.S. EPA 1993o	1.78E-03 [q]	Beyer et al. 1994
Short-tailed Shrew	F	1.50E-02	U.S. EPA 1993o	6.20E-01 [h]	U.S. EPA 1993o	1.51E-01 [l]	U.S. EPA 1993o	1.36E-02 [o]	Beyer et al. 1994
Spotted Sandpiper	SW, BR, FW	4.00E-02	U.S. EPA 1993o	5.69E-01 [f]	U.S. EPA 1993o; Nagy 1987	1.74E-01 [k]	U.S. EPA 1993o	4.15E-02 [u]	Beyer et al. 1994
Swift Fox	SG	1.40E+00	U.S. EPA 1993o	1.93E-01 [i]	U.S. EPA 1993o; Nagy 1987	9.34E-02 [l]	U.S. EPA 1993o	1.73E-03 [r]	Beyer et al. 1994
Western Meadow Lark	TG	9.00E-02	U.S. EPA 1993o	4.21E-01 [f]	U.S. EPA 1993o; Nagy 1987	1.31E-01 [k]	U.S. EPA 1993o	1.39E-02 [o]	Beyer et al. 1994

TABLE 5-1

INGESTION RATES FOR EXAMPLE MEASUREMENT RECEPTORS

Measurement Receptor	Example Food Web[a]	Body Weight (kg)	Reference	Food IR [e] (kg WW/ kg BW-day)	Reference	Water IR (L /kg BW-day)	Reference	Soil/Sed IR [m] (kg DW/ kg BW-day)	Reference
White-footed Mouse	SS	1.00E-02	U.S. EPA 1993o	6.14E-01 [g]	U.S. EPA 1993o; Nagy 1987	1.52E-01 [l]	U.S. EPA 1993o	2.70E-03	Beyer et al. 1994

Notes: IR- Ingestion Rate; WW- Wet weight; DW-Dry Weight; BW- Body Weight; kg - kilogram; L - Liter

a = Food Webs: BR - Brackish/Intermediate Marsh; F - Forest; FW - Freshwater/Wetland; SG - Shortgrass Prairie; SS - Shrub/Scrub; SW - Saltwater Marsh; TG - Tallgrass Prairie.

b = The body weight reported for the mallard is used as a surrogate value for the canvas back.

c = The body weight reported for the northern bobwhite is used as a surrogate value for the morning dove.

d = The body weight reported for the red-tailed hawk is used as a surrogate value for the northern harrier.

e = Food ingestion rate (IR) values are reported in Table 5-1 as kg WW/kg BW-day. To convert IR from a dry weight (as calculated using allometric equations) to a wet weight basis, the following general equation is used:

$$IR\ kg\ WW/kg\ BW\text{-}day = (IR\ kg\ DW/BW\text{-}day)/(1 - \%\ moisture/100)$$

Ingestion rate values provided in Table 5-1 are calculated based on assumed percent moisture content of food items of measurement receptors specified. For herbivores, the moisture content of ingested plant matter is assumed to be 88.0 percent (Taiz et al. 1991). For carnivores, the moisture content of ingested animal matter is assumed to be 68.0 percent (Sample et al. 1997). For omnivores, an equal fraction of plant and animal matter is assumed ingested with an overall average moisture content of 78.0 percent [(88.0 + 68.0)/2].

f = Food ingestion rates generated using the following allometric equation for all birds: IR (g/day) = 0.648 $Wt^{0.651}$ (g).

g = Food ingestion rates generated using the following allometric equation for rodents: IR (g/day) = 0.621 $Wt^{0.564}$ (g).

h = Allometric equations reported in U.S. EPA (1993o) do not represent intake rates for shrews; therefore, measured field values from the referenced sources are presented.

i = Food ingestion rates generated using the following allometric equation for all mammals: IR (g/day) = 0.235 $Wt^{0.822}$ (g).

j = Food ingestion rates generated using the following allometric equation for herbivores: IR (g/day) = 0.577 $Wt^{0.727}$ (g).

k = Water ingestion rates generated using the following allometric equation for all birds: IR (L/day) = 0.059 $Wt^{0.670}$ (kg).

l = Water ingestion rates generated using the following allometric equation for all mammals: IR (L/day) = 0.099 $Wt^{0.900}$ (kg).

m = Soil and sediment ingestion rates calculated based on percent soil in diet as reported in Beyer et al. 1994.

n = Percent soil in diet reported for the bald eagle is used as a surrogate value for the american kestrel, northern harrier, and red-tailed hawk.

o = Percent soil in diet is assumed as 10.0 percent of diet based on range presented in Beyer et al. 1994.

p	=	Percent soil in diet reported for the mallard is used as a surrogate value for the canvas back.
q	=	Percent soil in diet reported for the white-footed mouse is used as a surrogate value for the deer mouse and salt-marsh harvest mouse.
r	=	Percent soil in diet reported for the red fox is used as a surrogate value for the long-tailed weasel, mink, and swift fox.
s	=	Percent soil in diet is assumed as 2.0 percent of diet based on range presented for herbivores.
t	=	Percent soil in diet reported for the wild turkey is used as a surrogate value for the northern bobwhite.
u	=	Percent soil in diet reported for the western sandpiper is used as a surrogate value for the spotted sandpiper.

5.3.2 COPC Concentrations in Food Items of Measurement Receptors

Determination of COPC concentrations in food items is required for calculating the daily dose of COPC ingested for each class-specific guild measurement receptor being evaluated. Since the risk assessment considers potential future exposure that may occur as a result of facility emissions over time, these concentrations are generally expected to be estimated mathmatically. The following subsections provide guidance for estimating COPC concentrations in the following groups of food items:

- Invertebrates, phytoplankton, and rooted aquatic plants;
- Terrestrial plants;
- Fish; and
- Mammals, birds, reptiles, and amphibians.

5.3.2.1 COPC Concentration in Invertebrates, Phytoplankton, and Rooted Aquatic Plants

COPC concentrations in invertebrate, phytoplankton, and rooted aquatic plants can be calculated by rearranging the mathmatical expression for a bioconcentration factor (*BCF*). Equation 5-2 is the mathmatical definition of a *BCF*, which is the ratio, at steady-state, of the concentration of a compound in a food item to its concentration in a media. Equation 5-3 is the same equation expressed in terms of a COPC concentration in a food item.

$$BCF = \frac{C_i}{C_M} \qquad \text{Equation 5-2}$$

$$C_i = C_M \cdot BCF \qquad \text{Equation 5-3}$$

where

BCF	=	Bioconcentration factor (unitless [soil, sediment], or L/kg [water])
C_i	=	COPC concentration in *i*th plant or animal food item (mg COPC/kg)
C_M	=	COPC concentration in media (mg/kg [soil, sediment], or mg/L [water])

Equation 5-3 estimates a COPC concentration in an invertebrate, phytoplankton, and rooted aquatic plant to evaluate dose ingested to the measurement receptor. Calculation of COPC concentrations in media is further discussed in Chapter 3 and Appendix B. Media-to-receptor *BCF*s are receptor- and media-specific, and values along with supporting discussion are provided in Appendix C. Appendix F provides specific equations and supporting discussion for calculating COPC concentrations in plant and animal food items.

Equilibrium Partitioning (EqP) Approach

When adequate site-specific characterization data is available, specifically organic carbon fraction data for soil and sediment, the permitting authority may elect in some cases to allow the calculation of COPC concentrations in soil invertebrate (Connell and Markwell 1990) or sediment invertebrate (U.S. EPA 1993q) using the equilibrium partitioning (EqP) approach. However, the EqP approach is not prefered over use of measured BCF values multiplied by the COPC concentration in the media (i.e., sediment or soil), following the approach previously discussed.

The EqP approach utilizes the correlation of the concentrations of nonionic organic compounds in sediment, on an organic carbon basis, to their concentrations in the interstitial water, to determine the observed biological effects on sediment invertebrate (U.S. EPA 1993q). The EqP approach is only applicable for (1) hydrophobic nonionic organic compounds, (2) soil- and sediment-invertebrates, and (3) COPCs with empirical water bioconcentration factors (U.S. EPA 1993q). Also, the EqP approach assumes that the partitioning of the compound in sediment organic carbon and interstitial water are in equilibrium, and the sediment—interstitial water equilibrium system provides the same exposure as a water-only exposure (U.S. EPA 1993q).

To calculate the COPC concentration in an invertebrate using the EqP approach, the soil or sediment interstitial water concentration should be multiplied by the *BCF* determined from a water exposure for a benthic invertebrate:

$$C_I = C_{IW} \cdot BCF_{WI} \qquad \text{Equation 5-4}$$

where

C_I	=	COPC concentration in soil or benthic invertebrate (mg/kg)
C_{IW}	=	COPC concentration in soil or sediment interstitial water (mg/L)
BCF_{WI}	=	Bioconcentration factor for water-to-invertebrate (L/kg)

Equation 5-5 is used to calculate the COPC concentration in soil or sediment interstitial water for this approach:

$$C_{IW} = \frac{C_M}{f_{oc} \cdot K_{oc}} \qquad \text{Equation 5-5}$$

where

C_{IW}	=	COPC concentration in soil or sediment interstitial water (mg/L)
C_M	=	COPC concentration in media (mg/kg [soil, sediment])
f_{oc}	=	Fraction of organic carbon in soil or sediment (unitless)
K_{oc}	=	Organic carbon partitioning coefficient (L/kg)

5.3.2.2 COPC Concentration in Terrestrial Plants

The COPC concentration in terrestrial plants (C_{TP}) is calculated by summing the plant concentration due to direct deposition (*Pd*), air-to-plant transfer (*Pv*), and root uptake (*Pr*). Equation 5-6 should be used to compute a COPC concentration in terrestrial plants:

$$C_{TP} = Pd + Pv + Pr \qquad \text{Equation 5-6}$$

where

C_{TP}	=	COPC concentration in terrestrial plants (mg COPC/kg WW)
Pd	=	COPC concentration in plant due to to direct deposition (mg/kg WW)
Pv	=	COPC concentration in plant due to air-to-plant transfer (mg/kg WW)
Pr	=	COPC concentration in plant due to root uptake (mg/kg WW)

Calculation of *Pd*, *Pv*, and *Pr* is presented in Chapter 3 and Appendix B. Calculation of C_{TP} is further discussed in Appendix F.

5.3.2.3 COPC Concentration in Fish

The COPC concentration in fish is calculated by multiplying a COPC-specific *BCF* and trophic level-specific *FCM* by the dissolved water concentration, as follows:

$$C_F = BCF \cdot FCM \cdot C_{dw} \qquad \text{Equation 5-7}$$

where

C_F	=	COPC concentration in fish (mg/kg)
BCF	=	Bioconcentration factor for water-to-fish (L/kg)
FCM	=	Food-chain multiplier (unitless)
C_{dw}	=	Dissolved phase water concentration (mg/L)

The COPC concentration in fish is calculated using dissolved phase water concentrations, since bioconcentration, or estimated bioaccumulation, values are typically derived from studies based on dissolved phase water concentrations. The *FCM* used to calculate a COPC concentration in fish should be appropriate for the trophic level of the fish ingested by a measurement receptor. Development of *FCM* values is discussed in the following subsection, and actual recommended values are provided in Table 5-2. The dissolved phase water concentration is calculated as discussed in Chapter 3 and Appendix B. Values for bioconcentration factors for water-to-fish, and discussion on their determination, can be found in Appendix C. Calculation of C_F is further discussed in Appendix F.

Food-Chain Multipliers

*FCM*s presented in Table 5-2 were adopted directly from U.S. EPA (1995k), which determined them for K_{ow} values ranging from 3.5 through 9.0 using the Gobas (1993) model. U.S. EPA determined *FCM*s to develop water criteria protective to wildlife of the Great Lakes (U.S. EPA 1995j). As presented in Equation 5-8, U.S. EPA (1995k) calculated trophic level specific *FCM*s (see Table 5-2) utilizing *BAF* values obtained from the Gobas (1993) model and compound specific K_{ow} values.

$$FCM = \frac{BAF_l}{K_{ow}} \qquad \text{Equation 5-8}$$

where

FCM	=	Food-chain multiplier (unitless)
BAF_l	=	Bioaccumulation factor reported on a lipid-normalized basis using the freely dissolved concentration of a chemical in the water (L/kg)
K_{ow}	=	Octanol-water partition coefficient (L/kg)

BAF values predicted using the Gobas (1993) model were based on chemical concentrations in both the water column and surface sediment. Bioaccumulation values for fish were determined from the rate of chemical uptake, the rate of chemical depuration (including excretion), metabolism, and dilution due to growth. As reported in U.S.. EPA (1995k), data on physicochemical parameters and species characteristics reported by Oliver and Niimi (1988), Flint (1986), and Gobas (1993) were used.

For each K_{ow} value, the Gobas (1993) model reported correlating BAF_l values specific to each organism in the food web. U.S. EPA (1995k) determined trophic level-specific *FCM*s by calculating the geometric mean of the *FCM* for each organism in each respective trophic level. The *FCM*s were developed assuming no metabolism of a compound. Thus, for compounds where metabolism may occur (i.e., some PAHs), the COPC concentration in fish ingested by a measurement receptor may be overestimated. This information should be noted as an uncertainty in risk characterization. It should also be noted that the *FCM* values presented in Table 5-2 were developed using K_{ow} values reported in U.S. EPA (1995k); which may differ from K_{ow} values specified in Appendix A-2 of this guidance.

Using the U.S. EPA (1995k) assumption that a compound's log K_{ow} value approximates its BCF_l, Equation 5-8 for determining *FCM* values can also be expressed as follows:

$$FCM = \frac{BAF_l}{BCF_l} \qquad \text{Equation 5-9}$$

where

FCM	=	Food-chain multiplier (unitless)
BAF_l	=	Bioaccumulation factor reported on a lipid-normalized basis using the freely dissolved concentration of a chemical in the water (L/kg)
BCF_l	=	Bioconcentration factor reported on a lipid-normalized basis using the freely dissolved concentration of a chemical in the water (L/kg)

Equation 5-9 can also be written to demonstrate the relation of a *BCF* multiplied by a *FCM* to estimate a *BAF*, as shown in the following equation:

$$BAF = BCF \cdot FCM \qquad \text{Equation 5-10}$$

where

BAF	=	Bioaccumulation factor (L/kg)
BCF	=	Bioconcentration factor (L/kg)
FCM	=	Trophic level-specific food-chain multiplier (unitless)

*FCM*s are specified for use in this guidance to model a COPC concentration in fish, and also mammalian and bird food items, that are ingested by a measurement receptor. The *BCF-FCM* approach accounts for the uptake or bioaccumulation of COPCs into organisms, typically represented in equations as a *BAF* (U.S. EPA 1995j). The availability of data allows the *BCF-FCM* approach to be more consistently applied across class-specific guilds within food webs being evaluated.

U.S. EPA OSW recognizes the limitations and uncertainties of applying *FCM*s derived from aquatic food web data to terrestrial receptors, as well as all top level consumers, whether their food is chiefly aquatic or not. However, the *BCF-FCM* approach is recommended in this guidance because (1) evaluation of multiple food chain exposure pathways is typically required to estimate risk to multiple mammalian and avian guilds in several food webs, (2) screening level risk assessment results are intended to support develoment of permits and focus risk management efforts, rather than as a final point of departure for further evaluation, and (3) U.S. EPA OSW is aware of no other applicable multipathway approaches for consistently and reproducibly estimating COPC concentrations in prey ingested by upper-trophic-level ecological receptors, considering current data limitations. Therefore, U.S. EPA OSW believes the *BCF-FCM* approach is the best available quantitative method for estimating COPC concentrations in upper trophic level food items ingested by measurement receptors, considering data availabilty and the objectives inherent to a screening level risk assessment.

TABLE 5-2

FOOD-CHAIN MULTIPLIERS

Log K_{ow}	Trophic Level of Consumer		
	2	3	4
2.0	1.0	1.0	1.0
2.5	1.0	1.0	1.0
3.0	1.0	1.0	1.0
3.1	1.0	1.0	1.0
3.2	1.0	1.0	1.0
3.3	1.0	1.1	1.0
3.4	1.0	1.1	1.0
3.5	1.0	1.1	1.0
3.6	1.0	1.1	1.0
3.7	1.0	1.1	1.0
3.8	1.0	1.2	1.0
3.9	1.0	1.2	1.1
4.0	1.0	1.3	1.1
4.1	1.0	1.3	1.1
4.2	1.0	1.4	1.1
4.3	1.0	1.5	12
4.4	1.0	1.6	1.2
4.5	1.0	1.8	1.3
4.6	1.0	2.0	1.5
4.7	1.0	2.2	1.6
4.8	1.0	2.5	1.9
4.9	1.0	2.8	2.2
5.0	1.0	3.2	2.6
5.1	1.0	3.6	3.2
5.2	1.0	4.2	3.9
5.3	1.0	4.8	4.7
5.4	1.0	5.5	5.8
5.5	1.0	6.3	7.1
5.6	1.0	7.1	8.6

TABLE 5-2

FOOD-CHAIN MULTIPLIERS

Log K_{ow}	Trophic Level of Consumer		
	2	3	4
5.7	1.0	8.0	10
5.8	1.0	8.8	12
5.9	1.0	9.7	14
6.0	1.0	11	16
6.1	1.0	11	18
6.2	1.0	12	20
6.3	1.0	13	22
6.4	1.0	13	23
6.5	1.0	14	25
6.6	1.0	14	26
6.7	1.0	14	26
6.8	1.0	14	27
6.9	1.0	14	27
7.0	1.0	14	26
7.1	1.0	14	25
7.2	1.0	14	24
7.3	1.0	13	23
7.4	1.0	13	21
7.5	1.0	13	19
7.6	1.0	12	17
7.7	1.0	11	14
7.8	1.0	10	12
7.9	1.0	9.2	9.8
8.0	1.0	8.2	7.8
8.1	1.0	7.3	6.0
8.2	1.0	6.4	4.5
8.3	1.0	5.5	3.3
8.4	1.0	4.7	2.4
8.5	1.0	3.9	1.7
8.6	1.0	3.3	1.1

TABLE 5-2

FOOD-CHAIN MULTIPLIERS

Log K_{ow}	Trophic Level of Consumer		
	2	3	4
8.7	1.0	2.7	0.78
8.8	1.0	2.2	0.52
8.9	1.0	1.8	0.35
9.0	1.0	1.5	0.23

Source: U.S. EPA. 1995k. "Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation factors." EPA-820-B-95-005. Office of Water. Washington, D.C. March.

5.3.2.4 COPC Concentration in Mammals, Birds, Amphibians, and Reptiles

The COPC concentration in mammals and birds, as food items ingested by measurement receptors, are estimated using equations specific to each guild (i.e., herbivores, omnivores, and carnivores), and based on the plant and animal food items, and media ingested. Similar to calculating the COPC concentration in fish, a *BCF-FCM* approach is used to account for bioaccumulation. However, the contribution of COPC concentrations from each food item ingested must be accounted for directly for wildlife, whereas, the derivation of *BCF-FCM* values already accounts for the COPC contributions from all pathways for fish. Also for wildlife, a ratio of *FCM*s is applied to each animal food item ingested to account for the increase in COPC concentration occurring between the trophic level of the prey item (TLn) and the trophic level of the omnivore (TL3) or carnivore (TL4).

General equations for estimating COPC concentrations of food items in each guild, including use of a *FCM* ratio to estimate biomagnification, are described in the following subsections using mammals and birds as examples. Specific equations and discussion of associated parameters are provided in Appendix F. It should be noted that due to limited availabilty of biotransfer and toxicity data for reptiles and amphibians, the equations in the following subsections and in Appendix F have not been specifically described for use to model exposure to these receptors. However, if site-specific conditions and data warrant evaluation of reptiles and amphibians, the permitting authority may elect to utilize the same generic equations presented.

Herbivorous Mammals and Birds

As indicated in Equation 5-11, the COPC concentration in herbivorous mammals and birds is calculated by summing the contribution due to ingestion of contaminated plant food items and media. The general equation for computing COPC concentration in herbivores is as follows:

$$C_H = \sum(C_{Pi} \cdot BCF_{Pi-H} \cdot P_{Pi} \cdot F_{Pi}) + (C_{s/sed} \cdot BCF_{S/BS-H} \cdot P_{S/BS}) + (C_{wctot} \cdot BCF_{W-H} \cdot P_W) \quad \text{Equation 5-11}$$

where

C_H	=	COPC concentration in herbivore (mg/kg)
C_{Pi}	=	COPC concentration in *i*th plant food item (mg/kg)
BCF_{Pi-H}	=	Bioconcentration factor for plant-to-herbivore for *i*th plant food item (unitless)
P_{Pi}	=	Proportion of *i*th plant food item in diet that is contaminated (unitless)
F_{Pi}	=	Fraction of diet consisting of *i*th plant food item (unitless)
$C_{s/sed}$	=	COPC concentration in soil or bed sediment (mg/kg)
$BCF_{S/BS-H}$	=	Bioconcentration factor for soil-to-plant or bed sediment-to-plant (unitless)
$P_{S/BS}$	=	Proportion of soil or bed sediment in diet that is contaminated (unitless)
C_{wctot}	=	Total COPC concentration in water column (mg/L)
BCF_{W-HM}	=	Bioconcentration factor for water-to-herbivore (L/kg)
P_W	=	Proportion of water in diet that is contaminated (unitless)

Media-to-herbivore *BCF* values are COPC and receptor-specific and provided in Appendix C. As discussed in Appendix D, plant-to-herbivore *BCF* values are receptor-specific and determined from biotransfer factors. Calculation of COPC concentrations in plant food items and media is further discussed in previous sections of Chapter 5, and in Chapter 3 and Appendix B. The variables representing the diet fraction and proportion of diet contaminated are discussed in Section 5.3 and Appendix F. Appendix F also provides specific equations and supporting discussion for calculating the COPC concentration in herbivores.

Omnivorous Mammals and Birds

As indicated in Equation 5-12, the COPC concentration in omnivorous mammals and birds is calculated by summing the contribution due to ingestion of contaminated animal and plant food items, and media. However, unlike herbivores which are TL2 consumers, omnivores are TL3 consumers of animal food items and a ratio of *FCM*s is applied to each animal food item ingested to account for the increase in COPC concentration occurring between the trophic level of the prey item (TLn) and the trophic level of the omnivore (TL3). In general, the COPC concentration in omnivores depends on the COPC concentration in each food item ingested, and the trophic level of each food item, as follows:

$$C_{OM} = \sum \left(C_{Ai} \cdot \frac{FCM_{TL3}}{FCM_{TLn-Ai}} \cdot P_{Ai} \cdot F_{Ai} \right) + \sum \left(C_{Pi} \cdot BCF_{Pi-OM} \cdot P_{Pi} \cdot F_{Pi} \right) + \left(C_{s/sed} \cdot BCF_{S/BS-OM} \cdot P_{S/BS} \right) + \left(C_{wctot} \cdot BCF_{W-OM} \cdot P_{W} \right) \quad \text{Equation 5-12}$$

where

C_{OM}	=	COPC concentration in omnivore (mg/kg)
C_{Ai}	=	COPC concentration in *i*th animal food item (mg/kg)
FCM_{TL3}	=	Food chain multiplier for trophic level 3 (unitless)
FCM_{TLn-Ai}	=	Food chain multiplier for trophic level of *i*th animal food item (unitless)
P_{Ai}	=	Proportion of *i*th animal food item in diet that is contaminated (unitless)
F_{Ai}	=	Fraction of diet consiting of *i*th animal food item (unitless)
BCF_{Pi-OM}	=	Bioconcentration factor for plant-to-omnivore for *i*th plant food item (unitless)
C_{Pi}	=	COPC concentration in *i*th plant food item (mg/kg)
P_{Pi}	=	Proportion of *i*th plant food item that is contaminated (unitless)
F_{Pi}	=	Fraction of diet consiting of *i*th plant food item (unitless)
$C_{s/sed}$	=	COPC concentration in soil or bed sediment (mg/kg)
$BCF_{S/BS-OM}$	=	Bioconcentration factor for soil- or bed sediment-to-omnivore (unitless)
$P_{S/BS}$	=	Proportion of soil or bed sediment in diet that is contaminated (mg/kg)
C_{wctot}	=	Total COPC concentration in water column (mg/L)
BCF_{W-OM}	=	Bioconcentration factor for water-to-omnivore (L/kg)
P_{W}	=	Proportion of water in diet that is contaminated (unitless)

Media-to-omnivore *BCF* values are COPC and receptor-specific and provided in Appendix C. The use of an *FCM* ratio to estimate biomagnification between trophic levels is discussed in a following subsection.

Calculation of COPC concentrations in animal food items is further discussed in previous sections of Chapter 5. Calculation of COPC concentrations in plant food items and media is further discussed in previous sections of Chapter 5, and in Chapter 3 and Appendix B. The variables representing the diet fraction and proportion of diet contaminated are discussed in Section 5.3 and Appendix F. Appendix F also provides specific equations and supporting discussion for calculating the COPC concentration in omnivores.

Carnivorous Mammals and Birds

As indicated in Equation 5-13, the COPC concentration in carnivorous mammals and birds is calculated by summing the contribution due to ingestion of contaminated animal and media food items. In general, the equation for computing a COPC concentration for carnivorous food items is similar to the corresponding equation for omnivores; only without the component accounting for ingestion of plant food items. Similarly, a ratio of *FCM*s is applied to each animal food item ingested to account for the increase in COPC concentration occurring between the trophic level of the prey item (TLn) and the trophic level of the carnivore (TL4). The COPC concentration in carnivores depends on the COPC concentration in media, in each animal food item ingested, their respective trophic level, as follows:

$$C_C = \sum \left(C_{Ai} \cdot \frac{FCM_{TL4}}{FCM_{TLn-Ai}} \cdot P_{Ai} \cdot F_{Ai} \right) + \left(C_{s/sed} \cdot BCF_{S/BS-C} \cdot P_{S/BS} \right) + \left(C_{wctot} \cdot BCF_{W-C} \cdot P_W \right) \quad \text{Equation 5-13}$$

where

C_C	=	COPC concentration in carnivore (mg/kg)
C_{Ai}	=	COPC concentration in *i*th animal food item (mg/kg)
FCM_{TL3}	=	Food chain multiplier for trophic level 4 (unitless)
FCM_{TLn-Ai}	=	Food chain multiplier for trophic level of *i*th animal food item (unitless)
P_{Ai}	=	Proportion of *i*th animal food item in diet that is contaminated (unitless)
F_{Ai}	=	Fraction of diet consisting of *i*th animal food item (unitless)
$C_{s/sed}$	=	COPC concentration in soil or bed sediment (mg/kg)
$BCF_{S/BS-C}$	=	Bioconcentration factor for soil- or bed sediment-to-carnivore (unitless)

$P_{S/BS}$	=	Proportion of soil or bed sediment in diet that is contaminated (mg/kg)
C_{wctot}	=	Total COPC concentration in water column (mg/L)
BCF_{W-C}	=	Bioconcentration factor for water-to-carnivore (L/kg)
P_W	=	Proportion of water in diet that is contaminated (unitless)

Media-to-carnivore *BCF* values are COPC and receptor-specific and provided in Appendix C. The use of an *FCM* ratio to estimate biomagnification between trophic levels is discussed in the following subsection. Calculation of COPC concentrations in animal food items is further discussed in previous sections of Chapter 5. Calculation of COPC concentrations in plant food items and media is further discussed in previous sections of Chapter 5, and in Chapter 3 and Appendix B. The variables representing the diet fraction and proportion of diet contaminated are discussed in Section 5.3 and Appendix F. Appendix F also provides specific equations and supporting discussion for calculating the COPC concentration in carnivores.

Use of Food Chain Multiplier Ratio to Estimate Biomagnification

Biomagnification involves the transfer of a chemical in food through successive trophic levels (Hamelink et al. 1971). Chemicals with greatest potential to biomagnify are highly lipophillic, have low water solubilities, and are resistant to being metabolized (Metcalf et al. 1975). To account for COPC biomagnification in the food chain, U.S. EPA OSW recommends the use of *FCM* ratios as derived by U.S. EPA (1995k).

FCM ratios are used to estimate the increase in a COPC concentration resulting from the ingestion of TL2 prey (i.e., animal food item) by a TL3 measurement receptor (i.e., omnivore or carnivore), and the ingestion of TL2 and TL3 prey by a TL4 measurement receptor. Biomagnification, expressed as a biomagnification factor (*BMF*), equals the quotient of the *FCM* of the measurement receptor divided by the *FCM* of the prey. It is important to note that the basic difference between the *FCM* and *BMF* is that the *FCM*s relate back to trophic level one, whereas *BMF*s always relate back to the preceding trophic level (U.S. EPA 1995k). This relation is entirely compatible, but confusion can result if the terms specific to trophic level are not used consistently and clearly (U.S. EPA 1995k). As presented in U.S. EPA (1995k), the following relation of *FCM* to *BMF* can be expressed as follows:

$$BMF_{TL2} = FCM_{TL2} \qquad \text{Equation 5-14}$$

$$BMF_{TL3} = FCM_{TL3}/FCM_{TL2} \qquad \text{Equation 5-14A}$$

where

BMF_n = Biomagnification factor for *n*th trophic level
FCM_{TLn} = Food chain multiplier for *n*th trophic level

5.4 ASSESSMENT OF TOXICITY

Toxicity of a COPC is assessed by identifying toxicity reference values (*TRV*s) specific to a COPC and the measurement receptor being evaluated. As discussed in Chapter 6, *TRV*s are subsequently set as the denominator for computing COPC ecological screening quotients (*ESQ*s) during risk characterization. The available *TRV*s used in risk characterization for lower trophic level communities are media specific; whereas *TRV*s for upper trophic level class-specific guilds are provided in terms of dose ingested. *TRV*s for community and class-specific guild measurement receptors are further described below:

- Community (lower trophic level) *TRV*s are media specific and used to screen ecological effects to receptors inhabiting soil, surface water, and sediment. Community *TRV*s are expressed on a concentration basis, such as milligrams of COPC per kilogram of soil, and generally either:

  (1) a COPC media concentration that, based on its intended use by a regulatory agency, confers a high degree or protection to receptor populations or communities inhabiting the media (these include regulatory values such as federal ambient water quality criteria, state no-effect-level sediment quality guidelines, and sediment screening effect concenentrations), or

  (2) a laboratory-derived toxicity value representing a COPC media concentration that causes, over a chronic exposure duration, no adverse effects to a representative ecological receptor (e.g., no-observed-effect-concentration).

- Class-specific guild (upper trophic level) *TRV*s are used to screen ecological effects to wildlife, and expressed as a COPC daily dose ingested that causes, over a chronic exposure duration, no observed adverse effects to a measurement receptor. Class-specific guild *TRV*s are expressed in units of mass (e.g., milligrams or micrograms) of COPC per

kilogram body weight (wet weight) per day.

Guidance for selection of *TRV*s for community and class-specific guild measurement receptors is provided in the following sections. *TRV*s specific to example measurement receptors presented in the food webs in Chapter 4 are available in Appendix E.

5.4.1 General Guidance on Selection of Toxicity Reference Values

Compound specific *TRV*s should be identified for each measurement receptor evaluated to characterize risk to a community or class-specific guild. U.S. EPA OSW recommends evaluation of the following sources of toxicity values, listed in order of general preference, in determining *TRV*s for use in a screening level risk assessment:

Toxicity values developed and/or adopted by federal and/or state regulatory agencies; generally provided in the form of standards, criteria, guidance, or benchmarks. Toxicity values developed and/or adopted by federal or state regulatory agencies are generally media specific, and reported only for surface water and sediment. Examples include state or federal ambient water quality criteria (AWQC), National Oceanic and Atmospheric Administration (NOAA) effects range-low (ERL) values for sediment (Long et al. 1995), and State of Florida sediment quality guidelines (MacDonald 1993).

Toxicity values published in scientific literature. Appropriate values should be derived from a laboratory study which characterizes adverse effects on ecologically-relevant endpoints (e.g., growth, reproduction, mortality). As discussed in Section 5.4.1.3, toxicity values obtained from scientific literature may also require application of an uncertainty factor (UF) to account for extrapolation uncertainty.

Toxicity values calculated for sediment using equilibrium partitioning (EqP) approach. The EqP approach is further described in Section 5.3.2.1. Calculating sediment toxicity values using the EqP approach requires determination of (1) an organic carbon content of the sediments, and (2) a corresponding surface water toxicity value.

Toxicity values from surrogate compounds. Surrogate compounds are selected through evaluation of parameters such as chemical structure and toxicity mechanisms of action. For example, low molecular weight (i.e. those have two or less rings) polyaromatic hydrocarbons (PAH's) could be grouped together and evaluated using the toxicity data from a PAH congener belonging to this group.

The evaluation of toxicity values published in scientific literature should consider (1) ecological relevance of the study, (2) exposure duration (e.g., chronic, acute), and (3) study endpoints (e.g., NOAEL, LOAEL). The identification of literature toxicity values used to derive *TRV*s should focus on toxicological data

characterizing adverse effects on ecologically relevant endpoints, such as growth, seed germination, reproduction, and survival. Study endpoints specified for reported toxicity values generally include the following:

- Soil, surface water, and sediment measurement receptors
  - No-observed-effect-level (NOEL) or no-observed-effect-concentration (NOEC)
  - Lowest-observed-effect-level (LOEL) or lowest-observed-effect-concentration (LOEC)
  - Median lethal concentration to 50 percent of the test population (LC50) or median effective concentration for 50 percent of the test population (EC50)
- Wildlife measurement receptors
  - No-observed-adverse-effect-level (NOAEL)
  - Lowest-observed-adverse-effect-level (LOAEL)
  - Median lethal dose to 50 percent of the test population (LD50)

Evaluation of toxicity test data is further discussed in Section 5.4.1.1.

When multiple studies are assessed equally under the criteria above, professional judgement can be applied to determine the most appropriate study and corresponding toxicity value to be selected as the *TRV* (see Section 5.4.1.2). As discussed in Section 5.4.1.3, toxicity values obtained from scientific literature may also require application of an UF to account for extrapolation uncertainty (due to differences in test endpoint and exposure duration) when considering use of the test value as a *TRV* in a screening level risk assessment.

5.4.1.1 Evaluation of Toxicity Test Data

A *TRV* should represent a COPC concentration or dose that causes no observed adverse effects to an ecologically relevant endpoint of a receptor exposed for a chronic (long-term) duration. As noted above, evaluation of test data from ecologically relevant studies should be further assessed based on exposure duration and study endpoint.

The following hierarchy, in terms of decreasing preference, should be followed to assess exposure duration and study endpoint:

1. Chronic NOAEL
2. Subchronic NOAEL
3. Chronic LOAEL
4. Subchronic LOAEL
5. Acute median lethality point estimate
6. Single dose toxicity value

The following guidelines should be used to generally determine exposure duration:

- For fish, mammals, and birds:
  - A chronic test lasts for more than 90 days
  - A subchronic test lasts from 14 to 90 days
  - An acute test lasts less than 14 days
- For other receptors:
  - A chronic test lasts for 7 or more days
  - A subchronic test lasts from 3 to 6 days
  - An acute test lasts less than 3 days

The logic followed to identify the a toxicity value should be fully documented. Sources of toxicity values include electronic databases, reference compendia, and technical literature. Toxicity values identified from secondary sources should be verified, wherever possible, by reviewing the original study. If an original study is unavailable, or multiple studies of similar quality are available, best professional judgment should be used to determine an appropriate toxicity value.

5.4.1.2 Best Professional Judgement for Evaluating Toxicity Values

If more than one toxicity study meets a set of qualifying criteria applicable for study endpoint and exposure duration, best professional judgement should be used to identify the most appropriate study and corresponding toxicity value for *TRV* selection. The most appropriate study is the one with the least uncertainty about the accuracy of the value of endpoint (i.e., NOAEL) that, ultimately, provides the greatest degree of protectiveness to the applicable measurement receptor. The most appropriate study

should be identified by reviewing the experimental design of each study. Discussed below are important aspects of experimental design that should be evaluated.

- ***Number of treatments, spread between treatments, and number of replicates per treatment.*** The number of treatments and the spread between exposure concentrations (or dose groups) will affect the accuracy of the test endpoint (such as the NOAEL). That is, the smaller the spread between the NOAEL and LOAEL, the less the uncertainty is about the true concentration or dose at which there is no adverse effect. The statistical power of a toxicity test (or any test for that matter) is dependent, in large part, on the number of replicates (or number of animals per dose). That is, the ability of a test to detect statistical differences (test sensitivity) increases as the number of replicates increase.

- ***Exposure route.*** The exposure route of the test should coincide with the applicable exposure route or pathway under consideration in the risk assessment. For example, the screening level risk assessment may evaluate the risk of contaminated soils to terrestrial plants due to exposure to bulk soil. Therefore, a terrestrial plant toxicity study that evaluated the effects of soil solutions on a plant species may be a less appropriate than a study based on effects of bulk soil.

- ***Exposure during sensitive life stage.*** Ideally, all toxicity studies would evaluate the effects of a toxicant on the most sensitive life stage, such as neonatal zooplankton and first instar larvae. Therefore, the exposure duration should be receptor- and toxicant-specific.

- ***Nominal or measured test concentrations***. Measured test concentrations more accurately estimate the true concentration of a toxicant presented to a receptor. Nominal, or unmeasured, test concentrations do not account for potential losses of the toxicant (such as toxicant adsorbed to particulate material) or for inaccuracies in preparing test solutions. In addition, samples for measuring test concentrations should be collected from the exposure chamber, not the delivery system.

- ***Use, type, and performance of controls.*** A positive control (no toxicant) should be used in each toxicity study. The only difference between a positive control and a treatment is the absence of the toxicant from the control. Performance in a positive control should meet pre-existing performance criteria (such as acceptable survival). Treatment performance should be statistically compared to (or inferred from in some circumstances) to control performance to identify statistical endpoints (such as the NOAEL and LOAEL). In some situations, a negative control (toxicant with known toxicity, also called a performance control) may be appropriate. If a negative control is used, its results should be compared to standards to determine if test receptor sensitivity was acceptable.

- ***Method used to determine endpoint (i.e., NOAEL).*** Ideally, an acceptable number of replicates should be used so a test has statistical power. An appropriate statistical test should be performed to identify the NOAEL. In some cases, the NOAEL may have to be inferred because of insufficient number of replicates. While the latter is not unscientific, the former method provides a measure that the conclusion might be false. For example, if test results are statistically analyzed at a probability level of 95 percent, there is a 5 percent chance that the results of the statistical analysis are false.

5.4.1.3 Uncertainty Factors for Extrapolation From Toxicity Test Values to *TRV*s

Incomplete knowledge of the actual toxicity of a chemical leads to the use of UFs to reduce the likelihood that risk estimates do not underestimate risk. Historically, UFs have been used for various extrapolations, and their applications reflect policy to provide conservative estimates of risk (Chapman et al. 1998). As discussed below, UFs are used in the risk assessment to reduce the probability of underestimating ecological risk from exposures to combustor emissions. This is performed by multiplying a toxicity value by a UF to produce a *TRV* reflecting an NOAEL for a chronic exposure duration.

UFs should be used to convert a toxicity value to a chronic NOAEL-based *TRV*. In most cases, the UFs discussed below should be applicable to available toxicity values. In some cases, however, irregular toxicity data (such as, a subchronic LC50) may be the only available information. In these cases, the toxicity data should be thoroughly reviewed and professional judgment should be used to identify appropriate UFs that are consistent with those listed below. Special attention should be taken with toxicity values from single oral dose, intraperitoneal, and subchronic lethality tests.

Specifically, UFs should be used to account for extrapolation uncertainty due to differences in test endpoint and exposure duration:

- Test endpoint uncertainty—extrapolation from a non-NOAEL endpoint (e.g., LOAEL, LD50) to an NOAEL endpoint
- Duration uncertainty—extrapolation from a single dose, acute, or subchronic duration to a chronic duration

Except as noted above for irregular toxicity data, the following UFs (Calabrese and Baldwin 1993) should be used to convert a toxicity test endpoint to a *TRV* equivalent to a chronic NOAEL:

- A chronic LOAEL (or LOEL or LOEC) should be multiplied by a UF of 0.1 to convert it to a chronic NOAEL
- A subchronic NOAEL should be multiplied by a UF of 0.1 to convert it to a chronic NOAEL.
- An acute lethal value (such as an LC50 or LD50) should be multipled by an UF of 0.01 to convert it to a chronic NOAEL.

Chapter 6
Risk Characterization

What's Covered in Chapter 6:

- Risk Estimation
- Risk Description
- Uncertainty and Limitations of the Screening Level Risk Assessment

Risk characterization includes risk estimation and risk description (U.S. EPA 1992b). Risk estimation is an integration of the exposure assessment (see Section 5.1) and the toxicity assessment (see Section 5.4) to determine the potential risk to a community or guild from exposure to a COPC. Risk estimation is quantified using the quotient method to calculate an ecological screening quotient (*ESQ*) (Suter 1993). Risk description describes the magnitude and nature of potential risk for each community and guild, based on the quantitative results of the risk estimation and calculated *ESQ* values. Risk description also discusses the significance of the default assumptions used to assess exposure, because they affect the magnitude and certainty of the calculated *ESQ* value. The resultant risk characterization should consider any major uncertainties and limitations associated with results generated in performing the screening level risk assessment.

Section 6.1 discusses using the quotient method and calculation of *ESQ*s to estimate potential ecological risk. Section 6.2 discusses various aspects of the risk description. Section 6.3 discusses consideration of uncertainties and limitations.

6.1 RISK ESTIMATION

To estimate potential ecological risk, an *ESQ* should be calculated specific to each measurement receptor, COPC, and exposure scenario location evaluated in the risk assessment. Also, dietary-variable *ESQ*s should be computed for class-specific guild measurement receptors based on "equal diet" dose and "exclusive diet" dose, as discussed in Section 5.3. As expressed in Equation 6-1, an *ESQ* is the quotient of the COPC estimated exposure level (*EEL*) divided by the COPC and measurement receptor specific toxicity reference value (*TRV*), as follows:

$$ESQ = \frac{EEL}{TRV}$$ Equation 6-1

where

ESQ	=	Ecological screening quotient (unitless)
EEL	=	COPC estimated exposure level (mass COPC/mass media [communities] or mass daily dose COPC ingested/mass body weight-day [class-specific guilds])
TRV	=	COPC toxicity reference value (mass COPC/mass media [communities] or mass daily dose COPC ingested/mass body weight-day [class-specific guilds])

Care should be made to ensure that the units for the *EEL* value and the *TRV* are consistent, including correct use of corresponding wet and dry weights. *TRV*s specific to organic and inorganic compounds are typically expressed in units of µg/kg and mg/kg, respectively. General guidance for determining *TRV*s is provided in Chapter 5. Also, Appendix E provides compound specific *TRV*s for the example measurement receptors identified in the food webs in Chapter 4.

*ESQ*s for community measurement receptors are calculated using *EEL*s specific to the COPC concentration in the corresponding media. A COPC specific *ESQ* should be calculated for each community measurement receptor at each location evaluated, as appropriate for the food web being analyzed in the risk assessment. For calculating *ESQ*s for class-specific guild measurement receptors, the *EEL* is the daily dose of COPC ingested. A COPC specific *ESQ* should also be calculated for each class-specific guild measurement receptor at each location evaluated, as appropriate for the food web being analyzed in the risk assessment. For class-specific guild measurement receptors, *ESQ*s should be calculated specific to equal and exclusive diets (see Chapter 5).

To evaluate potential risk resulting from exposure of a measurement receptor to multiple COPCs at a specific location, each of the COPC-specific *ESQ* values should be summed to determine a total *ESQ*.

$$ESQ_{ReceptorTotal} = \Sigma\ ESQ_{COPC\ Specific}$$ Equation 6-2

where

$ESQ_{Receptor\ Total}$ = Total ecological screening quotient for receptor (unitless)
$ESQ_{COPC\ Specific}$ = COPC specific ecological screening quotient (unitless)

As for COPC-specific *ESQ*s, total *ESQ*s for class-specific guild measurement receptors should be calculated specific to equal and exclusive diets (see Chapter 5).

6.2 RISK DESCRIPTION

Risk description considers the magnitude and nature of potential risk for community and class-specific guild measurement receptors evaluated, and provides information for the risk manager and permitting authority to evaluate the significance of an *ESQ* value. Also, Section 6.2.2 recognizes some of the default exposure assumptions that may affect the magnitude of an *ESQ* value.

6.2.1 Magnitude and Nature of Ecological Risk

The magnitude and nature of potential risk should be further considered for each measurement receptor with a COPC-specific *ESQ* value equal to or above risk target levels specified by the appropriate permitting authority. Interaction between the risk assessor and the risk manager and permitting authority has been noted throughout the process (See Figure 1 for Scientific Management Decision Points). At the risk characterization phase of the risk assessment, most of the interaction between the risk assessor and the risk manager and permitting authority is through description of the certainty of the resulting risk estimates. Consistent with the NCP and current U.S. EPA guidance (1998c), the risk manager and permitting authority with input from the risk assessor should also consider the need to collect additional information to refine risk estimates and/or implement permit requirements (i.e., operating conditions, use of APCDs, waste feed conditions, or environmental monitoring) at combustion facilities where an *ESQ* exceeds risk target levels for ecological communities or guilds that may reasonably be expected to be exposed.

The magnitude and nature of potential risk should also be further considered for each measurement receptor with a total *ESQ* value greater than or equal to the target risk levels. While the total *ESQ* provides the risk manager and permitting authority with useful information regarding potential risk resulting from exposure of a measurement receptor to multiple COPCs at a specific location, potential limitations and uncertainties

associated with the calculation of the total *ESQ* should be considered before its use. Specifically, the resulting total *ESQ* is determined by summing COPC-specific *ESQ*s that will usually be calculated utilizing *TRV*s (see Chapter 5) based on different effects (e.g. growth, reproduction), toxicity endpoints (e.g., NOAEL, LOAEL) and/or exposure durations (e.g., chronic, acute). In considering usability of total *ESQ*s, U.S. EPA OSW recommends that the risk manager and permitting authority focus on the highest contributing COPCs, or classes of COPCs which can appropriately be added across effects, toxicity endpoints and exposure durations, in further evaluating potential risks due to exposure to multiple COPCs.

Broad assessment endpoints rather than toxicologically-specific endpoints are recommended for performing a screening level ecological risk assessment (see Chapter 5). Therefore, the potential risk to each community and guild evaluated in the risk assessment should be described. Specifically, potential adverse effects should be described for each community and guild with a COPC-specific or total *ESQ* value equal to or above risk target levels. This should be performed for each selected food web and receptor location evaluated, and specific to equal and exclusive diets for applicable class-specific guilds. The description should characterize potential risk to the selected assessment endpoints, based on the measures of effect and measurement receptors. U.S. EPA OSW recommends that the risk description specific to a measurement receptor include, at a minimum, the contributing COPCs, emission sources, exposure pathways, and significant uncertainties.

6.2.1.1 Target Levels

Target levels are risk management based and set by the regulatory authority. Target values are not a discrete indicator of observed adverse effect. If a calculated risk falls within target values, a regulatory authority may, without further investigation, conclude that a proposed action does not present an unacceptable risk. A calculated risk that exceeds these targets, however, would not, in and of itself, indicate that the proposed action is not safe or that it presents an unacceptable risk. Rather, a risk calculation that exceeds a target value triggers further careful consideration of the underlying scientific basis for the calculation.

6.2.2 Fate and Exposure Assumptions

As noted throughout this guidance, the screening level ecological risk assessment is based on numerous conservative assumptions affecting the potential for a receptor to be exposed to a compound emitted from a facility and the numeric magnitude of the resulting estimated risk. These fate and exposure assumptions are required as a result of current data gaps and uncertainties associated with available scientific information and data required for risk evaluation. However, U.S. EPA OSW recommends that as information is available to address data gaps and reduce uncertainties specific to ecological risks identified at a facility by the screening level risk assessment, it should be provided to the permitting authority for approval to be incorporated into evaluation of risk. Some of the fate and exposure assumptions utilized in this guidance to conduct a screening level risk assessment are listed below:

- The estimated COPC concentration in soil and sediment is 100 percent bioavailable. This includes a COPC that is weakly or strongly adsorbed to particles and a COPC that is dissolved in interstitial water.
- The estimated dissolved COPC concentration in the water column is 100 percent bioavailable. For ingestion of water by wildlife, this includes a COPC that is freely dissolved as an ion or compound, and a COPC that may be adsorbed to another matrix, such as dissolved organic carbon.
- The total COPC mass estimated to be ingested by a measurement receptor is taken up across the gut and reaches the site of toxic action. This includes COPC concentrations in food items and abiotic media. This assumes that no fraction of the COPC mass is metabolized or otherwise depurated by an ecological receptor, and that there is no competition for available sites where the toxic action occurs.
- The chemical species present is the most toxic form, and is the form represented by the *TRV*.
- Community measurement receptors inhabiting an abiotic medium take up 100 percent of the COPC concentration to which they are exposed. All COPC mass taken up by a plant or animal food item of a measurement receptor is assimilated into edible biomass.
- An ecological receptor is continuously exposed during its entire life, including critical life stage(s).
- A measurement receptor's home range is 100 percent within the assessment area being evaluated in the risk assessment.
- A measurement receptor's food is 100 percent contaminated.

The relevance of fate and exposure assumptions specific to COPCs at a site, and their numerical bias to resulting *ESQ* values should be considered before application of results. Also, to facilitate the qualitative assessment of toxicokinetic and toxicodynamic factors (e.g., bioavailability, metabolism), toxicological profiles of numerous compounds often considered in combustion risk assessments (see Section 2.3) are included in Appendix H. U.S. EPA OSW prepared these profiles because it believes that these compounds (1) will be the principal compounds of ecological concern at combustion facilities, and (2) to promote consistency in presenting and evaluating relevant COPC-specific toxicity information.

6.3 UNCERTAINTY AND LIMITATIONS OF THE RISK ASSESSMENT PROCESS

This section describes how to interpret uncertainties associated with the risk assessment. The discussion of uncertainties in this section and in Section 6.3.1 was adopted from the U.S. EPA *1996 Risk Assessment Support to the Development of Technical Standards for Emissions from Combustion Units Burning Hazardous Waste* (EPA Contract Number 68-W3-0028), dated February 20, 1996.

Uncertainty can be introduced into a risk assessment at every step of the process outlined in this document. Uncertainty occurs, because risk assessment is a complex process, requiring the integration of the following:

- Release of pollutants into the environment
- Fate and transport of pollutants, in a variety of different and variable environments, by processes that are often poorly understood or too complex to quantify accurately
- Potential for adverse effects in receptors, as extrapolated from studies of differing species
- Probability of adverse effects in functionality of food web that is made up of species that are highly variable

Uncertainty is inherent in the process even if the most accurate data with the most sophisticated models are used. The methodology outlined in this document relies on a combination of point values—some conservative and some typical—yielding a point estimate of exposure and risk that falls at an unknown percentile of the full distributions of exposure and risk. For this reason, the degree of conservatism in risk estimates cannot be known; instead, it is known that the values combine many conservative factors and are likely to overstate actual risk (Hattis and Burmaster 1994). Therefore, a formal uncertainty analysis is

required to determine the degree of conservatism. This section discusses the types of uncertainty and the areas in which uncertainty can be introduced into an assessment. In addition, this section discusses methods for qualitatively and quantitatively addressing uncertainty in risk assessments.

It should also be noted, variability is often used interchangeably with the term "uncertainty," but this is not strictly correct. Variability may be tied to variations in physical and biological processes, and cannot be reduced with additional research or information, although it may be known with greater certainty (for example, the weight distribution of a species may be known and represented by the mean weight and its standard deviation). "Uncertainty" is a description of the imperfect knowledge of the true value of a particular variable or its real variability in an individual or a group. In general, uncertainty is reducible by additional information-gathering or analysis activities (that is, better data or better models), whereas real variability will not change (although it may be more accurately known) as a result of better or more extensive measurements (Hattis and Burmaster 1994).

6.3.1 Types of Uncertainty

Finkel (1990) classified all uncertainty into four types: (1) variable uncertainty, (2) model uncertainty, (3) decision-rule uncertainty, and (4) variability. Variable uncertainty and model uncertainty are generally recognized by risk assessors as major sources of uncertainty; decision rule is of greatest concern to the risk manager.

6.3.1.1 Variable Uncertainty

Variable uncertainty occurs when variables appearing in equations cannot be measured precisely or accurately, because of either (1) equipment limitations, or (2) spatial or temporal variances between the quantities being measured. Random, or sample, errors are common sources of variable uncertainty that are especially critical for small sample sizes. It is more difficult to recognize nonrandom, or systematic, errors that result from the basis for sampling, experimental design, or choice of assumptions. As stated in Section 6.3, true variability is something we can not do much about (except to know that it exists).

6.3.1.2 Model Uncertainty

Model uncertainty is associated with all models used in all phases of a risk assessment. For example, the use of a single species to represent several will introduce uncertainty into the risk assessment because of the considerable amount of interspecies variability in sensitivity to a COPC. Computer models are simplifications of reality, requiring exclusion of some variables that influence predictions but cannot be included in models because of (1) increased complexity, or (2) a lack of data for these variables. The risk assessor needs to consider the importance, in consultation with the modeler, of excluded variables on a case-by-case basis. In addition, a model which was developed to use "average" conditions as its inputs, could result in a large amount of uncertainty when "specific" conditions are used. Finally, choosing the correct model form is often difficult, because conflicting theories appear to explain a phenomenon equally well.

The models specified for use in this document were selected on the basis of scientific policy. Therefore, the air dispersion and deposition model (ISCST3) and the indirect exposure models (IEM) were selected, because they provide the information needed to conduct indirect assessments and are considered by U.S. EPA to be state-of-the-science models. This choice of models could also be considered under decision rule uncertainty. ISCST3—the air dispersion model recommended for use—has not been widely applied in its present form. Few data are available on atmospheric deposition rates for chemicals other than criteria pollutants, thereby making it difficult to (1) select input variables related to deposition, and (2) validate modeled deposition rates. Because dry deposition of vapor phase materials is evaluated external to the air dispersion model, the plume is not depleted and, as a result, mass balance is not maintained. The effect of this would be to overestimate deposition, but the magnitude of the overestimation is unknown. Mass balance is maintained for other forms of deposition (such as wet deposition and particle phase dry deposition). Long-range transport of pollutants into and out of the areas considered was not modeled, resulting in an underestimation of risk attributable to each facility.

In addition to air dispersion modeling, the use of other fate and transport models recommended by this guidance can also result in some uncertainty. For example, the models which estimate COPC concentrations in waterbodies may be particularly conservative for waterbodies located in estuarine environments with tidal influence. Because tidal influence is not considered in the models presented in Chapter 3, the resultant dilution of COPC concentrations in water and sediments likely caused by tidal

influence will not be considered in the risk assessment. Thus, the risk assessment results will likely be more conservative for tidally influenced waterbodies than for those waterbodies that are not tidally influenced. Permitting decisions based on risk estimates for estuarine environments should consider this uncertainty. The delineation of this uncertainty may be one area that could be addressed in a more refined site-specific risk assessment, if warranted.

6.3.1.3 Decision-rule Uncertainty

Decision-rule uncertainty is probably of greatest concern to risk managers. This type of uncertainty arises, for example, out of the need to balance different social concerns when determining an acceptable level of risk. The uncertainty associated with risk analysis influences many policy and risk management decisions. Possibly the most important aspect for the risk estimates is the selection of constituents to be included in the analysis. Constituents identified by this guidance will include compounds that have the potential to pose the greatest risk to ecological receptors through exposure. For example, many PICs are highly lipophilic and tend to bioaccumulate, thereby presenting a potentially high risk to upper trophic level receptors through the consumption of contaminated food items.

6.3.2 Description of Qualitative Uncertainty

Often, sources of uncertainty in a risk assessment can be determined but cannot be quantified. For example, this can occur when a factor is known or expected to be variable, but no data are available (e.g., presence of COPCs without toxicity data). In this case, default data may be available that can be useful in estimating a possible range of values. Uncertainty also often arises out of a complete lack of data. A process may be so poorly understood that the uncertainty cannot be quantified with any confidence. In addition, some sources of uncertainty (such as uncertainty in theories used to deduce models) are inherent qualifications reflecting subjective modes of confidence rather than probabilistic arguments. When uncertainty can be presented only qualitatively, the possible direction and orders of magnitude of the potential error should be considered.

6.3.3 Description of Quantitative Uncertainty

Knowledge of experimental or measurement errors can also be used to introduce a degree of quantitative information into a qualitative presentation of uncertainty. For example, standard laboratory procedures or field sampling methods may have a known error level that can be used to quantify uncertainty. In many cases, uncertainty associated with particular variable values or estimated risks can be expressed quantitatively and further evaluated with variations of sensitivity analyses. Finkel (1990) identified a six-step process for producing a quantitative uncertainty estimate:

- Define the measure of risk (i.e., assessment endpoint). More than one measure of risk may result from a particular risk assessment: however, the uncertainty should be quantified or reached individually.
- Specify "risk equations" that present mathematical relationships that express the risk measure in terms of its components. This step is used to identify the important variables in the risk estimation process.
- Generate an uncertainty distribution for each variable or equation component. These uncertainty distributions may be generated by using analogy, statistical inference techniques, expert opinion, or a combination of these.
- Combine the individual distributions into a composite uncertainty distribution.
- Recalibrate the uncertainty distributions. Inferential analysis could be used to "tighten" or "broaden" particular distributions to account for dependencies among the variables and to truncate the distributions to exclude extreme values.
- Summarize the output clearly, highlighting the important risk management implications. Address specific critical factors.
    - Implication of supporting a point estimate produced without considering uncertainty
    - Balance of the costs of under- or over-estimating risks
    - Unresolved scientific controversies, and their implications for research

When a detailed quantitative treatment of uncertainty is required, statistical methods are employed. Two approaches to a statistical treatment of uncertainty with regard to variable values are described here and were used in this analysis where appropriate. The first is to use an appropriate statistic to express all variables for which uncertainty is a major concern. For example, if a value used is from a sample (such as

yearly emissions from a stack), the mean and standard deviation should both be presented. If the sample size is very small, it may be appropriate to (1) give the range of sample values and use a midpoint as a best estimate in the model, or (2) use the smallest and largest measured value to obtain two estimates that bound the expected true value. Selection of the appropriate statistic depends on the amount of data available and the degree of detail required. Uncertainties can be propagated by using analytical or numerical methods.

A second approach is to use the probability distributions of major variables to propagate variable value uncertainties through the equations used in a risk analysis. A probability distribution of expected values is then developed for each variable value. These probability distributions are typically expressed as either probability density functions (*PDF*) or cumulative probability density functions (*CPF*). The *PDF* presents the relative probability for discrete variable values, whereas the *CPF* presents the cumulative probability that a value is less than or equal to a specific value.

A composite uncertainty distribution is created by combining the individual distributions with the equations used to calculate the probability of particular adverse effects and points. Numerical or statistical methods are often used. In Monte Carlo simulations, for example, a computer program is used to repeatedly solve the model equations, under different selections of variable values, to calculate a distribution of exposure (or risk) values. Each time the equations are calculated, values are randomly sampled from the specified distributions for each variable. The end result is a distribution of exposure (or risk). These can again be expressed as *PDF*s or, more appropriately, as *CPF*s. The distribution enables the risk assessor to choose the value corresponding to the appropriate percentile in the overall distribution. For example, the risk assessor can select an exposure level or risk level that corresponds to the 95th percentile of the overall risk distribution rather than a point estimate of risk that is based on the 95th percentile values for each variable.

6.3.4 Risk Assessment Uncertainty Discussion

The science of risk assessment is evolving; where the science base is incomplete and uncertainties exist, science policy assumptions must me made. It is important for risk assessments of facilities that burn hazardous waste to fully explain the areas of uncertainty in the assessments and to identify the key assumptions used in conducting the assessments. Toward that end, a table should be added to the end of each section (e.g., stack emissions, air modeling, exposure assessment, risk characterization) which lists the

key assumptions in that section, the rationale for those assumptions, their effect on estimates of risk (overestimation, underestimation, neutral), and the magnitude of the effect (high, medium, low). For example, it could explain that using a particular input variable, such as exit gas temperature, will under- or overestimate long-term emissions, and the resulting risks, by a factor of *x*. These tables can be used to evaluate the extent to which protective assumptions were used in the risk assessments. They can also help determine the nature of the uncertainty analysis to be performed. The assumptions listed in the risk characterization section, which synthesizes the data outputs from the exposure and toxicity analyses, should be the most significant assumptions from each of the previous sections.

Within this guidance, identification of uncertainties and limitations are also included with the discussion of specific technical issues (e.g., TOE, estimates of emission rates, COPC selection process, quantification of non-detects) as they are presented in their respective sections. Limitations associated with parameter values and inputs to equations are presented in the Appendices.

As an example discussion, the following summarizes some of the uncertainty involved in the air dispersion modeling component of the risk assessment process.

Although dispersion modeling is a valuable tool for estimating concentration and deposition impacts, it has many limitations. The accuracy of the models is limited by (1) the ability of the model algorithms to depict atmospheric transport and dispersion of contaminants, and (2) the accuracy and validity of the input data. For example, most refined models require input of representative meteorological data from a single measuring station. In reality, a release will encounter highly variable meteorological conditions that are constantly changing as it moves downwind. U.S. EPA's *Guideline on Air Quality Models—Revised* (Title 51 CFR Appendix W) describes two types of model uncertainty. Inherent uncertainty involves deviations in concentrations that occur even if all of the model input is accurate. Reducible uncertainty is associated with the model and the uncertain input values that will affect the results. Although it is important to accurately represent actual conditions by selecting the right model, and using accurate and representative input data, all model results are subject to uncertainty. Nevertheless, models are generally considered reasonably reliable in estimating the magnitude of highest concentrations resulting from a release, although they may not necessarily be time-and space-specific (Title 51 CFR Appendix W). When applied properly, air dispersion models are typically accurate to ± 10 to 40 percent and can be used to yield a "best estimate" of air concentrations (Title 51 CFR Appendix W).

Uncertainties specific to other technical components (e.g., TOE, quantification of non-detects) of the risk assessment process are further described in their respective chapters or sections of this guidance.

6.3.5 Limitations and Uncertainties Specific to a Screening Level Ecological Risk Assessment

As a screening-level tool, the screening level ecological risk assessment has several inherent limitations. Some of these limitations are discussed in Section 6.3.5.1. After computing the *ESQ*s and analyzing the risk assessment results, the risk assessor should evaluate the uncertainty associated with the screening level risk assessment. Section 6.3.5.2 provides a list of uncertainties that U.S. EPA OSW recommends should typically be evaluated, at least qualitatively, in a screening level risk assessment.

6.3.5.1 Limitations Typical of a Screening Level Ecological Risk Assessment

The approach used to select the measurement receptors is based, in part, on the premise that if key components of the ecosystem are protected, protection will be conferred to populations and, by extension, communities and the ecosystem. Although this approach is reasonable given the nature of the analysis and the availability of the data, protection of measurement receptors may not always adequately protect all ecologically significant assessment endpoints. Similarly, the selection process for ecological receptors relies on a modified trophic element approach. As a result, representative species may not be the most sensitive to particular compounds, but may have been chosen as a function of their ecological significance and the availability of natural history information.

COPCs were selected to provide a conservative representation of those compounds in hazardous waste combustion stack and fugitive emissions that have the highest potential to result in adverse ecological effects. Due to a lack of data on adverse ecological effects associated with combustion emissions through all exposure pathways, this list may not be all inclusive.

The toxicity of compounds varies with the measurement receptors and with the availability and form of a given compound. If a compound is more bioavailable to an organism for absorption or uptake (such as through increased solubility in the surface soil, surface water, or sediment), then the toxic potential of the compound increases. Availability and chemical form are affected by factors such as pH, temperature, alkalinity, seasonal variation, microbial activity, organic carbon content, and complexation with other

compounds. In the risk assessment, bioavailability of COPCs is assumed to be similar to that observed in the toxicity studies reported in the literature. Thus, toxicity may be over- or underestimated, depending in part on the extent to which site-specific compound bioavailability differs from those in studies reported in the literature.

Attempts to quantify and correct for uncertainty resulting from the use of surrogate species is common, but controversial. Calabrese and Baldwin (1993) discuss the use of uncertainty factors to adjust for extrapolations among taxa, between laboratory and field responses, and between acute and chronic responses. These multipliers are expected to adjust for differences in responses among taxa resulting from differences in physiology and metabolism. When extrapolating from laboratory to field settings, important considerations are differences in physical environment, organism behavior, and interactions with other ecological components. Extrapolation between responses will be necessary in some cases, particularly when data on relevant endpoints are not available (most commonly when extrapolating from a LOAEL to a NOAEL). The net effect of uncertainty factors on the accuracy of the risk assessment depends on the accuracy of the assumptions that underlie the factors themselves.

6.3.5.2 Uncertainties Typical of a Screening Level Ecological Risk Assessment

A screening level risk assessment is typically performed using at least some default parameter values in place of site-specific measured data (see Sections 3.12 and 6.2.2), and incorporating assumptions (see Section 6.2) as a result of data gaps. The absence of site-specific information and the need to use these assumptions may result in uncertainty associated with the calculation of *ESQ*s. An understanding of the uncertainties associated with the *ESQ*s is necessary for understanding the significance of the *ESQ*s. After identifying the major uncertainties associated with the risk assessment results, their significance should be evaluated with respect to the computed *ESQ*s. Uncertainties that generally should be evaluated in a screening level ecological risk assessment for a combustion facility are listed below:

- Changes in future COPC emissions compared with modeled emission rates used in the risk assessment.
- Quantification of emissions and evaluation of non-detects used in the risk assessment.
- The site-specific representativeness of food web(s) used in the risk assessment.

- The exposure potential of the measurement receptors.
- The representativeness of equal and exclusive diet assumptions for measurement receptors.
- The effect of COPC physicochemical properties on estimates of fate and bioavailability.
- The effect of site-specific environmental conditions affecting the fate, transport, and bioavailability of the COPCs.
- The assumption that once exposed, a measurement receptor does not metabolize or eliminate a COPC.
- The potential risk to measurement receptors of COPCs with no *TRV*s.

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Screening Level Ecological Risk Assessment Protocol for Hazardous Waste Combustion Facilities

Volume Two
Appendix A

Peer Review Draft

APPENDIX A

CHEMICAL-SPECIFIC DATA

Screening Level Ecological Risk Assessment Protocol

August 1999

A-1 CHEMICALS FOR CONSIDERATION AS COMPOUNDS OF POTENTIAL CONCERN

A-2 COMPOUND SPECIFIC PARAMETER VALUES

APPENDIX A-1

INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

TABLE A-1
INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994a) for Risk Assessments	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994b)	PICs in Stack Emissions Actually Detected
50-00-0	Formaldehyde (methylene oxide)	K009, K010, K038, K040, K156, K157	X		X	X	
50-06-6	Phenobarbital						
50-07-7	Mitomycin						
50-18-0	Cyclophosphamide						
50-29-3	4,4'-DDT		X				
50-32-8	Benzo(a)pyrene	F032, F034, F037, F038, K001, K022, K035, K141, K142, K144, K145, K147, K148	X		X	X	X
50-55-5	Reserpine						
51-28-5	2,4-Dinitrophenol	K001	X			X	
51-43-4	Epinephrine						
51-52-5	Propylthiouracil						
51-79-6	Ethyl carbamate (urethane)					X	
52-85-7	Famphur						
53-70-3	Dibenzo(a,h)anthracene	F032, F034, K022, K141, K142, K144, K145, K147, K148	X			X	
53-96-3	2-Acetylaminofluorene						
54-11-5	Nicotine						
55-18-5	Nitrosodiethylamine						
55-38-9	Fenthion						
55-63-0	Nitroglycerine						
55-91-4	Diisopropylfluorophosphate (DFP)						
56-04-2	Methylthiouracil						

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

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56-23-5	Carbon tetrachloride	F001, F024, F025, K016, K019, K020, K021, K073, K116, K150, K151, K157	X		X	X	X
56-38-2	Parathion						
56-49-5	3-Methylcholanthrene						
56-53-1	Diethylstilbestrol						
56-55-3	Benzo(a)anthracene	F032, F034, K001, K022, K035, K141, K142, K143, K144, K145, K147, K148	X		X	X	
56-57-5	Nitroquinoline-1-oxide						
56-72-4	Coumaphos						
57-12-5	Cyanide		X				X
57-14-7	1,1-Dimethyl hydrazine	K107, K108, K109, K110					
57-24-9	Strychnine		X			X	
57-41-0	5,5-Diphenylhydantoin						
57-57-8	beta-Propiolactone						
57-74-9	Chlordane	K097	X			X	
57-97-6	7,12-Dimethylbenz(a)anthracene						
58-89-9	gamma-BHC (Lindane)						
58-89-9	Lindane (all isomers)					X	
58-90-2	2,3,4,6-Tetrachlorophenol	F020, F023, F027, F028, K001	X				
59-50-7	4-Chloro-3-methylphenol (p-chloro-m-cresol)	F004, K001					
59-89-2	N-Nitrosomorpholine						
60-09-3	Aminoazobenzene						
60-11-7	Dimethyl aminoazobenzene					X	

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60-34-4	Methyl hydrazine						
60-35-5	Acetamide						
60-51-5	Dimethoate						
60-57-1	Dieldrin		X				
61-82-5	Amitrole						
62-38-4	Phenylmercury acetate						
62-44-2	Phenacetin						
62-50-0	Ethyl methanesulfonate		X			X	
62-53-3	Aniline	K083, K103, K104, K112, K113	X			X	
62-55-5	Thioacetamide						
62-56-6	Thiourea						
62-73-7	Dichlorovos		X				
62-74-8	Fluoroacetic acid, sodium salt						
62-75-9	N-Nitrosodimethylamine						
63-25-2	Carbaryl	K156					
64-17-5	Ethanol						
64-18-6	Formic acid (methanoic acid)	K009, K010	X			X	
64-64-7	Di-n-propylnitrosamine					X	
64-67-5	Diethyl sulfate						
65-85-0	Benzoic acid		X				X
66-27-3	Methyl methanesulfonate						
66-75-1	Uracil mustard						

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67-56-1	Methanol		X				
67-64-1	Acetone		X				X
67-66-3	Chloroform (trichloromethane)	F024, F025, K009, K010, K019, K020, K021, K029, K073, K116, K149, K150, K151, K158	X		X	X	X
67-72-1	Hexachloroethane (perchloroethane)	F024, F025, K016, K030, K073	X		X	X	
68-12-2	Dimethyl formamide						
70-25-7	N-Methyl-N'-nitro-N-nitrosoguanidine (MNNG)						
70-30-4	Hexachlorophene		X			X	
71-43-2	Benzene	F005, F024, F025, F037, F038, K085, K104, K105, K141, K142, K143, K144, K145, K147, K151, K159	X		X	X	X
71-55-6	Methyl chloroform (1,1,1-trichloroethane)	F001, F002, F024, F025, K019, K020, K028, K029, K096			X	X	X
72-20-8	Endrin		X				
72-33-3	Mestranol						
72-43-5	Methoxychlor		X			X	
72-54-8	4,4'-DDD		X				
72-55-9	DDE		X			X	
72-57-1	Trypan blue						
74-83-9	Bromomethane (methylbromide)	K131, K132	X		X	X	X
74-87-3	Chloromethane (methyl chloride)	F024, F025, K009, K010, K149, K150, K157	X		X	X	X
74-88-4	Methyl iodide (Iodomethane)						
74-90-8	Hydrogen cyanide	K011, K013					

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74-93-1	Thiomethanol						
74-95-3	Methylene bromide		X		X	X	
74-97-5	Bromochloromethane				X	X	X
75-00-3	Chloroethane		X			X	
75-01-4	Vinyl chloride	F024, F025, K019, K020, K028, K029	X		X	X	X
75-05-8	Acetonitrile	K011, K013, K014	X		X		
75-07-0	Acetaldehyde		X			X	
75-09-2	Methylene chloride	F001, F002, F024, F025, K009, K010, K156, K157, K158	X			X	X
75-15-0	Carbon disulfide	F005	X		X	X	X
75-21-8	Ethylene oxide		X			X	
75-25-2	Bromoform		X			X	X
75-27-4	Bromodichloromethane		X		X	X	X
75-29-6	2-Chloropropane		X			X	
75-34-3	1,1-Dichloroethane	F024, F025	X		X	X	X
75-35-4	1,1-Dichloroethene	F024, F025, K019, K020, K029	X		X	X	
75-36-5	Acetyl chloride						
75-44-5	Phosgene (hydrogen phosphide)	K116				X	
75-45-6	Chlorodifluoromethane		X				X
75-55-8	1,2-Propylenimine (2-methyl aziridine)						
75-56-9	Propylene oxide						
75-60-5	Cacodylic acid						

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75-69-4	Trichlorofluoromethane (Freon 11)	F001, F002	X			X	X
75-70-7	Trichloromethanethiol						
75-71-8	Dichlorodifluoromethane		X			X	
75-86-5	2-Methylactonitrile						
75-87-6	Chloral						
76-01-7	Pentachloroethane	F024, F025					X
76-13-1	1,1,2-Trichloro-1,2,2-trifluoroethane(Freon 113)	F001, F002	X			X	X
76-44-8	Heptachlor	K097	X			X	
77-47-4	Hexachlorocyclopentadiene	F024, F025, K032, K033, K034	X			X	X
77-78-1	Dimethyl sulfate	K131				X	
78-00-2	Tetraethyl lead						
78-32-0	Tri-p-tolyl phosphate						
78-34-2	Dioxathion						
78-59-1	Isophorone		X				
78-83-1	Isobutyl alcohol	F005					
78-87-5	1,2-Dichloropropane		X			X	X
78-93-3	2-Butanone (methyl ethyl ketone)	F005	X		X	X	X
78-97-7	2-Hydroxypropionitrile						
79-00-5	1,1,2-Trichloroethane	F002, F024, F025, K019, K020, K095, K096	X		X	X	X
79-01-6	Trichloroethene	F001, F002, F024, F025, K018, K019, K020	X		X	X	X
79-06-1	Acrylamide	K014					

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79-10-7	Acrylic acid						
79-11-8	Chloroacetic acid						
79-19-6	Thiosemicarbazide						
79-20-9	Methyl acetate		X				
79-22-1	Methyl chlorocarbonate						
79-34-5	1,1,2,2-Tetrachloroethane	F024, F025, K019, K020, K030, K073, K095, K150	X		X	X	
79-44-7	Dimethyl carbamoyl chloride						
79-46-9	2-Nitropropane	F005					
80-62-6	Methyl methacrylate						
81-07-2	Saccharin						
81-81-2	Warfarin						
82-68-8	Pentachloronitrobenzene (PCNB)		X			X	
83-32-9	Acenaphthene	K022	X				
84-66-2	Diethyl phthalate		X			X	X
84-74-2	Dibutyl phthalate		X		X	X	X
85-01-8	Phenanthrene	K022					
85-44-9	Phthalic anhydride (1,2-benzenedicarboxylic anhydride)	K023, K024, K093, K094	X			X	
85-68-7	Butylbenzyl phthalate		X		X	X	X
86-30-6	N-Nitrosodiphenylamine		X				
86-50-0	Azinphos-methyl						
86-73-7	Fluorene	K022	X		X		

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

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86-88-4	alpha-Naphthylthiourea						
87-65-0	2,6-Dichlorophenol	K043					
87-68-3	Hexachlorobutadiene (perchlorobutadiene)	F024, F025, K016, K018, K030	X		X	X	X
87-86-5	Pentachlorophenol	F021, F027, F028, F032, K001	X		X	X	X
88-06-2	2,4,6-Trichlorophenol	F020, F023, F027, F028, K001, K043, K099, K105	X		X	X	X
88-74-4	o-Nitroaniline (2-nitroaniline)					X	
88-75-5	2-Nitrophenol						X
88-85-7	Dinoseb						
90-04-0	o-Anisidine					X	
90-13-1	1-Chloronaphthalene						
91-20-3	Naphthalene	F024, F025, F034, K001, K022, K035, K060, K087, K145	X		X	X	X
91-22-5	Quinoline		X			X	
91-57-6	2-Methylnaphthalene						
91-58-7	2-Chloronaphthalene		X			X	
91-59-8	2-Naphthylamine (beta-naphthylamine)						
91-80-5	Methapyrilene						
91-94-1	3,3'-Dichlorobenzidine		X			X	
92-52-4	Biphenyl		X		X	X	
92-67-1	4-Aminobiphenyl						
92-87-5	Benzidine		X				
92-93-3	4-Nitrobiphenyl						

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TABLE A-1
INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

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93-72-1	Silvex	F027					
94-58-6	Dihydrosaffrole						
94-59-7	Safrole (5-(2-Propenyl)-1,3-benzodioxole)		X			X	
94-75-7	2,4-D		X			X	
95-06-7	Sulfallate						
95-47-6	o-Xylene (dimethyl benzene)		X		X	X	X
95-48-7	o-Cresol	F004	X			X	
95-50-1	1,2-Dichlorobenzene	F002, F024, F025, K042, K085, K105	X		X	X	X
95-53-4	o-Toluidine	K112, K113, K114	X			X	
95-57-8	2-Chlorophenol	K001	X			X	X
95-79-4	5-Chloro-2-methylaniline						
95-80-7	2,4-Toluene diamine	K112, K113, K114, K115, K027					
95-83-0	4-Chloro-1,2-phenylenediamine						
95-94-3	1,2,4,5-Tetrachlorobenzene	K085, K149, K150, K151	X		X	X	X
95-95-4	2,4,5-Trichlorophenol	F020, F023, F027, F028, K001	X		X	X	
96-09-3	Styrene oxide						
96-12-8	1,2-Dibromo-3-chloropropane		X		X	X	
96-18-4	1,2,3-Trichloropropane		X			X	
96-23-1	1,3-Dichloro-2-propanol						
96-45-7	Ethylene thiourea	K123, K124, K125, K126	X			X	
97-63-2	Ethyl methacrylate		X			X	
98-01-1	Furfural		X			X	

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98-07-7	Benzotrichloride	K015, K149	X			X	
98-82-8	Cumene		X		X	X	X
98-83-9	Methyl styrene (mixed isomers)		X			X	
98-86-2	Acetophenone		X			X	X
98-87-3	Benzal chloride						
98-95-3	Nitrobenzene	F004, K083, K103, K104	X			X	
99-09-2	3-Nitroaniline						
99-35-4	1,3,5-Trinitrobenzene		X			X	
99-55-8	5-Nitro-o-toluidine						
99-59-2	5-Nitro-o-anisidine						
99-65-0	1,3-Dinitrobenzene	K025	X			X	
100-01-6	4-Nitroaniline (p-nitroaniline)						
100-02-7	4-Nitrophenol (p-nitrophenol)					X	
100-25-4	1,4-Dinitrobenzene (p-dinitrobenzene)		X			X	
100-41-4	Ethylbenzene		X		X	X	X
100-42-5	Styrene		X		X	X	
100-44-7	Benzyl chloride	K015, K085, K149	X		X	X	
100-51-6	Benzyl alcohol						
100-52-7	Benzaldehyde		X		X	X	X
100-75-4	N-Nitrosopiperidine						
101-05-3	Anilazine						
101-14-4	4,4'-Methylenebis (2-chloroaniline)						

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101-27-9	Barban						
101-55-3	4-Bromophenyl phenyl ether						
101-61-1	4,4'-Methylenebis (N,N-dimethylaniline)						
101-68-8	Methylene diphenyl diisocyanate (MDI)						
101-79-9	4,4-Methylenedianiline					X	
101-80-4	4,4'-Oxydianiline						
102-82-9	Tributylamine						
103-33-3	Azobenzene		X		X	X	
103-85-5	Phenylthiourea						
105-60-2	Caprolactam						
105-67-9	2,4-Dimethylphenol	K001	X			X	X
106-42-3	p-Xylene (dimethyl benzene)				X	X	X
106-44-5	p-Cresol (4-methyl phenol)	F004	X			X	
106-46-7	1,4-Dichlorobenzene	F024, F025, K085, K105, K149, K150	X		X	X	X
106-47-8	p-Chloroaniline		X			X	
106-49-0	p-Toluidine	K112, K113, K114	X			X	
106-50-3	p-Phenylenediamine						
106-51-4	Quinone					X	
106-88-7	1,2-Epoxybutane						
106-89-8	Epichlorohydrin (1-chloro-2,3 epoxypropane)	K017	X			X	
106-93-4	Ethylene dibromide	K117, K118, K136	X			X	
106-99-0	1,3-Butadiene				X	X	

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107-02-8	Acrolein		X			X	
107-05-1	Allyl chloride	F024, F025					
107-06-2	1,2-Dichloroethane (ethylene dichloride)	F024, F025, K018, K019, K020, K029, K030, K096	X		X	X	X
107-07-3	2-Chloroethanol						
107-10-8	n-Propylamine						
107-12-0	Propionitrile						
107-13-1	Acrylonitrile	K011, K013	X		X	X	
107-18-6	Allyl alcohol						
107-19-7	Propargyl alcohol		X			X	
107-20-0	Chloroacetaldehyde	K010					
107-21-1	Ethylene glycol (1,2-ethanediol)		X			X	
107-30-2	Chloromethyl methyl ether						
107-49-3	Tetraethyl pyrophosphate						
107-98-2	Propylene glycol monomethyl ether		X			X	
108-05-4	Vinyl acetate		X			X	
108-10-1	Methyl isobutyl ketone		X			X	X
108-18-9	Diisopropylamine						
108-31-6	Maleic anhydride	K023, K093					
108-38-3	m-Xylene (dimethyl benzene)		X		X	X	X
108-39-4	m-Cresol	F004	X			X	
108-46-3	Resorcinol						

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108-60-1	bis (2-Chloroisopropyl)ether					X	
108-67-8	1,3,5-Trimethylbenzene		X				X
108-87-2	Methylcyclohexane					X	
108-88-3	Toluene	F005, F024, F025, K015, K036, K037, K149, K151	X		X	X	X
108-90-7	Chlorobenzene	F002, F024, F025, K015, K105, K149	X		X	X	X
108-95-2	Phenol	K001, K022, K087	X		X	X	X
108-98-5	Thiophenol (benzenethiol)						
109-06-8	2-Picoline	K026					
109-77-3	Malononitrile		X			X	
109-88-4	2-Methoxyethanol		X			X	
109-89-7	Diethylamine						
109-99-9	Tetrahydrofuran		X				X
110-54-3	n-Hexane		X			X	
110-75-8	2-Chloroethylvinyl ether						
110-80-5	Ethylene glycol monoethyl ether	F005	X			X	
110-86-1	Pyridine	F005, K026, K157	X			X	
111-15-9	Ethylene glycol monoethyl ether acetate					X	
111-42-2	Diethanolamine						
111-44-4	bis(2-chloroethyl)ether	K017	X		X	X	
111-54-6	Ethylene(bis)dithiocarbamic acid						
111-76-2	Ethylene glycol monobutyl ether					X	
111-91-1	bis(2-chloroethoxy)methane				X	X	

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114-26-1	Propoxur (Bayton)						
115-02-6	Azaserine						
115-29-7	Endosulfan		X				
115-90-2	Fensulfothion						
116-06-3	Aldicarb						
117-79-3	2-Aminoanthraquinone						
117-80-6	Dichlone						
117-81-7	bis(2-ethylhexyl)phthalate		X		X	X	X
117-84-0	Di-n-octylphthalate		X			X	
118-74-1	Hexachlorobenzene (perchlorobenzene)	F024, F025, K016, K018, K030, K042, K085, K149, K150, K151	X		X	X	X
118-96-7	2,4,6-Trinitrotoluene		X				
119-90-4	3,3'-Dimethoxybenzidine		X			X	
119-93-7	3,3'-Dimethylbenzidine						
120-12-7	Anthracene	K022	X		X	X	
120-58-1	Isosafrole						
120-62-7	Piperonyl sulfoxide						
120-71-8	p-Cresidine						
120-80-9	Catechol						
120-82-1	1,2,4-Trichlorobenzene	F024, F025, K085, K150	X		X	X	X
120-83-2	2,4-Dichlorophenol	K043, K099	X		X	X	
121-14-2	2,4-Dinitrotoluene	K025, K111	X			X	

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121-44-8	Triethylamine	K156, K157					
121-69-7	N,N-Diethyl aniline						
121-75-5	Malathion		X				
122-09-8	a,a-Dimethylphenethylamine						
122-39-4	Diphenylamine	K083, K104	X			X	
122-66-7	1,2-Diphenylhydrazine		X			X	
123-31-9	Hydroquinone						
123-33-1	Maleic hydrazide		X			X	
123-38-6	Propionaldehyde					X	
123-63-7	Paraldehyde	K009, K010, K026					
123-91-1	Dioxane (1,4-dioxane)		X		X	X	
124-48-1	Chlorodibromomethane		X				X
126-68-1	0,0,0-Triethyl phosphorothioate						
126-72-7	tris(2,3-dibromopropyl) phosphate						
126-75-0	Demeton-S						
126-98-7	Methacrylonitrile		X			X	
126-99-8	Chloroprene						
127-18-4	Tetrachloroethene (Perchloroethylene)	F001, F002, F024, F025, K016, K019, K020, K073, K116, K150, K151	X		X	X	X
129-00-0	Pyrene	K022	X		X		X
130-15-4	1,4-Naphthoquinone	K024					
131-11-3	Dimethyl Phthalate		X		X	X	

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131-89-5	2-Cyclohexyl-4,6-dinitro-phenol		X				
131-89-5	2-Cycloyhexyl-4,6-dinitrophenol					X	
132-32-1	3-Amino-9-ethylcarbazole						
132-64-9	Dibenzofuran				X		
133-06-2	Captan				X		
133-90-4	Chloramben						
134-32-7	1-Naphthylamine (alpha-naphthylamine)						
137-17-7	2,4,5-Trimethylaniline						
137-26-8	Thiram						
140-57-8	Aramite						
140-88-5	Ethyl acrylate						
141-66-2	Dicrotophos						
143-33-9	Sodium cyanide	F007, F008, F009, F010, F011					
143-50-0	Kepone						
145-73-3	Endothall		X			X	
148-82-3	Melphalan						
151-50-8	Potassium cyanide	F007, F008, F009, F010, F011					
151-56-4	Ethylene imine (Aziridine)						
152-16-9	Octamethyl pyrophosphoramide						
156-60-5	(trans)1,2-dichloroethene	F024, F025	X			X	
156-62-7	Calcium cyanamide						
189-55-9	Dibenzo(a,i)pyrene						

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191-24-2	Benzo(g,h,i)perylene	K022			X	X	
192-65-4	Dibenzo(a,e)pyrene						
192-97-2	Benzo(e)pyrene	K022				X	
193-39-5	Indeno(1,2,3-cd)pyrene	F032, F034, K001, K022, K035, K141, K142, K147, K148	X			X	
205-82-3	Benzo(j)fluoranthene	K022			X	X	
205-99-2	Benzo(b)fluoranthene (3,4-Benzofluoranthene)	K001, K022, K035, K141, K142, K143, K144, K147, K148	X		X	X	
206-44-0	Fluoranthene	K001, K022, K035	X		X	X	X
207-08-9	Benzo(k)fluoranthene	F034, K022, K141, K142, K143, K144, K147, K148	X		X	X	
208-96-8	Acenaphthalene	K001, K022, K035					
218-01-9	Chrysene	F037, F038, K001, K022, K035	X		X	X	
224-42-0	Dibenz(a,j)acridine						
225-51-4	Benz[c]acridine						
297-97-2	O,O-Diethyl O-pyrazinyl phosphorothioate						
297-97-2	Thionazine						
298-00-0	Methyl parathion		X				
298-02-2	Phorate	K038, K040	X				
298-03-3	Demeton-O						
298-04-4	Disulfoton		X				
299-84-3	Ronnel		X				
300-76-5	Naled		X				

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302-01-2	Hydrazine						
302-17-0	Chloral hydrate						
303-34-1	Lasiocarpine						
305-03-3	Chlorambucil						
309-00-2	Aldrin		X				
311-45-5	Diethyl-p-nitrophenyl phosphate						
315-18-4	Mexacarbate						
319-84-6	alpha-Hexachlorocyclohexane (alpha-BHC)	F024	X			X	
319-85-7	beta-Hexachlorocyclohexane (beta-BHC)		X			X	
319-86-8	delta-BHC						
321-60-8	2-Fluorobiphenyl						
334-88-3	Diazomethane						
353-50-4	Carbon oxyfluoride						
357-57-3	Brucine						
367-12-4	2-Fluorophenol						
460-00-4	4-Bromofluorobenzene						
460-19-5	Cyanogen (oxalonitrile)		X			X	
463-58-1	Carbonyl sulfide						
465-73-6	Isodrin						
470-90-6	Chlorfenvinphos						
479-45-8	Tetryl						
492-80-8	Auramine						

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494-03-1	Chlornaphazin						
504-24-5	4-Aminopyridine						
505-60-2	Mustard gas						
506-61-6	Potassium silver cyanide	F006, F007, F008, F009, F010, F011, F012, F019, K007, K088					
506-64-9	Silver cyanide	F006, F012, F019, K007, K088					
506-68-3	Cyanogen bromide (bromocyanide)		X			X	
506-77-4	Cyanogen chloride		X			X	
510-15-6	Chlorobenzilate		X			X	
512-56-1	Trimethyl phosphate						
528-29-0	1,2-Dinitrobenzene (o-Dinitrobenzene)		X			X	
532-27-4	2-Chloroacetophenone					X	
534-52-1	4,6-Dinitro-o-cresol	F004				X	
540-36-3	1,4-Difluorobenzene						
540-73-8	1,2-Dimethylhydrazine					X	
540-84-1	2,2,4-Trimethylpentane					X	
541-53-7	Dithiobiuret						
541-73-1	1,3-Dichlorobenzene	F024, F025, K085, K105				X	X
542-62-1	Barium cyanide						
542-75-6	1,3-Dichloropropene		X			X	
542-76-7	3-Chloropropionitrile						
542-88-1	bis(Chloromethyl)ether	K017	X		X	X	

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544-92-3	Copper cyanide						
557-19-7	Nickel cyanide						
557-21-1	Zinc cyanide						
563-12-2	Ethion						
563-68-8	Thallium(I)acetate						
584-84-9	2,4-Toluene diisocyanate	K027				X	
590-60-2	Bromoethene					X	
591-08-2	1-Acetyl-2-thiourea						
591-78-6	2-Hexanone (butyl methyl ketone)						
592-01-8	Calcium cyanide						
593-60-2	Vinyl bromide						
598-31-2	Bromoacetone						
602-87-9	5-Nitroacenaphthene						
606-20-2	2,6-Dinitrotoluene		X			X	
608-93-5	Pentachlorobenzene	F024, F025, K085, K149, K150, K151	X		X	X	X
615-53-2	N-Nitroso-N-methylurethane						
621-64-7	N-Nitroso-di-n-propylamine		X				
623-40-5	Toluene-2,6-diamine		X			X	
624-83-9	Methyl isocyanate					X	
628-86-4	Mercury fulminate						
630-10-4	Selenourea						
630-20-6	1,1,1,2-Tetrachloroethane	F024, F025, K019, K020, K030, K095	X		X	X	

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636-21-5	o-Toluidine hydrochloride						
640-19-7	Fluoroacetamide						
680-31-9	Hexamethylphosphoramide						
684-93-5	N-Nitroso-N-methylurea						
692-42-2	Diethylarsine						
696-28-6	Dichlorophenylarsine						
732-11-6	Phosmet						
755-04-5	Titanium tetrachloride						
757-58-4	Hexaethyl tetraphosphate						
759-73-9	N-Nitroso-N-ethylurea						
764-41-0	1,4-Dichloro-2-butene					X	
765-34-4	Glycidylaldehyde		X			X	
786-19-6	Carbophenothion						
822-06-0	Hexamethylene-1,5-diisocyanate					X	
924-16-3	N-Nitroso-di-n-Buetylamine		X			X	
930-55-2	N-Nitrosopyrrolidine						
959-98-8	Endosulfan I						
961-11-5	Tetrachlorvinphos						
1024-57-3	Heptachlor epoxide		X				
1031-07-8	Endosulfan sulfate						
1116-54-7	N-Nitrosodiethanolamine						
1120-71-4	1,3-Propane sultone					X	

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1303-28-2	Arsenic pentoxide						
1314-32-5	Thallic oxide						
1314-62-1	Vanadium pentoxide						
1319-77-3	Cresols/cresylic acid (isomers and mixtures)	F004					
1327-53-3	Arsenic trioxide						
1330-20-7	Xylene (total)		X		X		X
1332-21-4	Asbestos						
1335-32-6	Lead subacetate						
1336-36-3	Polychlorinated biphenyls (209 congeners)		X		X	X	X
1338-23-4	2-Butanone peroxide						
1464-53-5	1,2,3,4-Diepoxybutane						
1563-66-2	Carbofuran	K156, K158					
1582-09-8	Trifluralin						
1615-80-1	N,N'-Diethylhydrazine						
1634-04-4	Methyl tert butyl ether					X	
1718-51-0	Terphenyl-d14						
1746-01-6	2,3,7,8-Tetrachlorodibenzo(p)dioxin (TCDD)	F020, F022, F023, F026, F027, F028, F032	X		X	X	X
1836-75-5	Nitrofen						
1888-71-7	Hexachloropropene						
2037-26-5	Toluene-d8						
2104-64-5	EPN						

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

TABLE A-1
INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994a) for Risk Assessments	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994b)	PICs in Stack Emissions Actually Detected
2303-16-4	Diallate (cis or trans)						
2310-17-0	Phosalone						
2385-85-5	Mirex						
2425-06-1	Captafol						
2763-96-4	5-(Aminomethyl)-3-isoxazolol						
2921-88-5	Chlorpyrifos		X				
3114-55-4	Chlorobenzene-d5						
3288-58-2	O,O-Diethyl S-methyl dithiophosphate						
3689-24-5	Tetraethyl dithiopyrophosphate						
4170-30-3	Crotonaldehyde (Propylene aldehyde)		X			X	
4549-40-0	N-Nitrosomethylvinylamine						
5131-60-2	4-Chloro-1,3-phenylenediamine						
5344-82-1	1-(o-Chlorophenyl)thiourea						
6533-73-9	Thallium(I)carbonate						
6923-22-4	Monocrotophos						
6959-48-4	3-(Chloromethyl)pyridine hydrochloride						
7005-72-3	4-Chlorophenyl phenyl ether	F020, F023, F027, F028					
7421-93-4	Endrin aldehyde						
7439-92-1	Lead	F035, F037, F038, K002, K003, K005, K046, K048, K049, K051, K052, K061, K062, K064, K069, K086, K100	X		X	X	X
7439-96-5	Manganese				X		X
7439-97-6	Mercury	K071, K106	X		X	X	X

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

TABLE A-1
INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

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7440-02-0	Nickel	F006	X		X	X	X
7440-22-4	Silver		X		X	X	
7440-28-0	Thallium		X		X	X	
7440-36-0	Antimony	K021, K161	X		X	X	
7440-38-2	Arsenic	F032, F034, F035, K031, K060, K084, K101, K102, K161	X		X	X	X
7440-39-3	Barium		X		X	X	
7440-41-7	Beryllium		X			X	X
7440-43-9	Cadmium	F006, K061, K064, K069, K100	X		X	X	X
7440-47-3	Chromium (total)	F032, F034, F035, F037, F038, K090			X	X	X
7440-48-4	Cobalt						
7440-50-8	Copper						X
7440-62-2	Vanadium						
7440-66-6	Zinc				X		X
7446-18-6	Thallium(I)sulfate						
7487-94-7	Mercuric chloride		X				
7488-56-4	Selenium sulfide						
7647-01-0	Hydrogen Chloride (hydrochloric acid)		X				X
7664-38-2	Phosphoric acid						
7664-39-3	Hydrogen fluoride						X
7664-41-7	Ammonia		X			X	X
7700-17-6	Crotoxyphos						

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

TABLE A-1
INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994a) for Risk Assessments	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994b)	PICs in Stack Emissions Actually Detected
7723-14-0	Phosphorus						
7778-39-4	Arsenic acid						
7782-41-4	Fluorine						
7782-49-2	Selenium		X		X	X	
7782-50-5	Chlorine		X				
7783-00-8	Selenium dioxide						
7783-06-4	Hydrogen sulfide						
7786-34-7	Mevinphos						
7791-12-0	Thallium(I)chloride						
7803-51-2	Phosphine						
7803-55-6	Ammonium vanadate						
8001-35-2	Toxaphene (chlorinated camphene)	K041, K098					
8065-48-3	Demeton						
10102-43-9	Nitric oxide						
10102-44-0	Nitrogen dioxide						X
10102-45-1	Thallium(I)nitrate						
10595-95-6	N-Nitrosomethylethylamine						
11096-82-5	Arochlor-1260						
11097-69-1	Arochlor-1254		X				
11104-28-2	Arochlor-1221						
11141-16-5	Arochlor-1232						
12039-52-0	Thallium(I)selenite						

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

TABLE A-1
INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994a) for Risk Assessments	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994b)	PICs in Stack Emissions Actually Detected
12672-29-6	Arochlor-1248						
12674-11-2	Arochlor-1016		X				
13071-79-9	Terbufos						
13171-21-6	Phosphamidon						
13463-39-3	Nickel carbonyl						
13765-19-0	Calcium chromate						
16752-77-5	Methomyl						
18540-29-9	Chromium (hexavalent)	F006, F019, K002, K003, K004, K005, K006, K007, K008, K048, K049, K050, K051, K061, K062, K069, K086, K100	X		X		X
18883-66-4	Streptozotocin						
19408-74-3	1,2,3,7,8,9-Hexachlorodibenzo(p)dioxin	F021, F022, F026, F027, F028, F032			X	X	
20816-12-0	Osmium tetroxide						
20830-81-3	Daunomycin						
20859-73-8	Aluminum phosphide						
21609-90-5	Leptophos						
22967-92-6	Methyl mercury		X		X	X	
23950-58-5	Pronamide		X			X	
25013-15-4	Methyl styrene		X				
25265-76-3	Phenylenediamine	K083, K103, K104					
25376-45-8	Toluenediamine						
26471-62-5	Toluene diisocyanate						
33213-65-9	Endosulfan II						

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

TABLE A-1
INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994a) for Risk Assessments	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994b)	PICs in Stack Emissions Actually Detected
33245-39-5	Fluchloralin						
35822-46-9	1,2,3,4,6,7,8-Heptachlorodibenzo(p)dioxin	F032			X	X	
39196-18-4	Thiofanox						
39227-28-6	1,2,3,4,7,8-Hexachlorodibenzo(p)dioxin	F021, F022, F026, F027, F028, F032			X	X	
39300-45-3	Dinocap						
40321-76-4	1,2,3,7,8-Pentachlorodibenzo(p)dioxin	F020, F021, F022, F023, F026, F027, F028, F032			X	X	X
53469-21-9	Arochlor-1242						
53494-70-5	Endrin ketone						
55673-89-7	1,2,3,4,7,8,9-Heptachlorodibenzofuran	F032			X	X	
57117-41-6	2,3,4,7,8-Pentachlorodibenzofuran	F020, F021, F022, F023, F026, F027, F028, F032			X	X	X
57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	F021, F022, F026, F027, F028, F032			X	X	
57653-85-7	1,2,3,6,7,8,-Hexachlorodibenzo(p)dioxin	F021, F022, F026, F027, F028, F032			X	X	
60851-34-5	2,3,4,6,7,8-Hexachlorodibenzofuran	F021, F022, F026, F027, F028, F032			X	X	
67562-39-4	1,2,3,4,6,7,8-Heptachlorodibenzofuran	F032			X	X	
70648-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran	F021, F022, F026, F027, F028, F032			X		
72918-21-9	1,2,3,7,8,9-Hexachlorodibenzofuran	F021, F022, F026, F027, F028, F032			X	X	
109719-77-9	1,2,3,7,8-Pentachlorodibenzofuran	F020, F021, F022, F023, F026, F027, F028, F032			X	X	X
125322-32-9	2,3,7,8-Tetrachlorodibenzofuran	F020, F022, F023, F026, F027, F028, F032			X	X	X
--	Beryllium compounds						
--	Cadmium compounds						
--	Chlorocyclopentadiene				X	X	
--	N-Chlorodiisopropyl amine						

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

TABLE A-1
INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994a) for Risk Assessments	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994b)	PICs in Stack Emissions Actually Detected
--	N-Chloroisopropyl amine						
--	Chromium compounds						
--	Creosote	K001, K035					
--	Cyanide compounds	F006, F007, F008, F009, F010, F011, F012, F019, K007, K060, K088					
--	O-Decyl hydroxylamine						
--	Dibenzo(a,e)fluoranthene	K022			X	X	
--	Dibenzo(a,h)fluoranthene	K022			X	X	
--	Dibutylchloramine						
--	3,3-Dichloroisopropyl ether						
--	Dichloropentadiene					X	
--	Dimethylnitrosamine					X	
--	Lead compounds						
--	Nicotine salts						
--	2-Nitrodiphenylamine						
--	Octachlorodibenzo(p)dioxin				X	X	
--	Octachlorodibenzofuran				X	X	
--	Phthalic acid esters						
--	Saccharin salts						
--	Sodium O-ethylmethylphosphonate Diisopropylamine						
--	Strychnine salts						
--	Thioamine						

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

TABLE A-1
INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994a) for Risk Assessments	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994b)	PICs in Stack Emissions Actually Detected
--	O-decyl-hydroxylamine						
--	Acenaphthene-d10						
--	Antimony compounds						
--	Arsenic compounds (inorganic, including arsine)						
--	2-Chloro-1,3-butadiene	F024, F025					
--	Chrysene-d12						
--	Cobalt compounds						
--	Coke oven emissions						
--	Dibenz(a)anthracene	K001, K035					
--	1,4-Dichlorobenzene-d4						
--	Dichloroethylene	K073					
--	Dichloropropane	F024, F025					
--	Dichloropropanols	K017					
--	Dichloropropene	F024, F025					
--	Manganese compounds						
--	Mercury compounds						
--	Naphthalene-d8						
--	Nickel compounds						
--	Nitrobenzene-d5						
--	Perylene-d12						
--	Phenanthrene-d10						

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

TABLE A-1
INFORMATION ON COMPOUNDS OF POTENTIAL INTEREST

CAS Number	Compound Name	Compounds Listed in 40 CFR Part 261 Appendix VII or VIII	Chemical-Specific Data Available	PICs Recommended by U.S. EPA (1994a) for Risk Assessments	U.S. EPA Compounds Identified in Combustion Unit Emissions (1993)	U.S. EPA Recommended and Potential PICs (1994b)	PICs in Stack Emissions Actually Detected
--	Phenol-d6						
--	Phenolic compounds	K060					
--	Phosphorodithioic and phosphorothioic acid esters	K036, K037, K038, K039, K040					
--	2,3,7,8-substituted Polychlorinated dibenzo(p)dioxin congeners (2,3,7,8-PCDDs)						
--	2,3,7,8-substituted Polychlorinated dibenzofuran congeners (2,3,7,8-PCDFs)						
--	Selenium compounds						
--	Tetrachlorobenzene	F024, F025					
--	2,4,6-Tribromophenol						
--	Trichloropropane	K017					

Note: See Table A-1 References and Discussion (Appendix A-1) for explanation of the information presented.

APPENDIX A-1

COMPOUNDS OF POTENTIAL INTEREST

REFERENCES AND DISCUSSION

This discussion lists reference documents for each of the columns in Table A1-1 and briefly describes the quality of data associated with these references. This information is only presented for informational purposes to assist in planning data collection.

A1.1 COLUMN 1: CHEMICAL ABSTRACTS SERVICE (CAS) NUMBER

The CAS number is a unique number assigned to each compound in the table. Compounds are listed by CAS number, in ascending order, to prevent problems with alphabetization procedures or differences in common nomenclature.

A1.2 COLUMN 2: COMPOUND NAME

The most common compound name is listed. Where appropriate, common synonyms are also listed to aid the user in identifying particular compounds.

A1.3 COLUMN 3: COMPOUNDS LISTED IN 40 CFR PART 261 APPENDIX VII OR VIII

Appendix VII of Title 40 Code of Federal Regulations (40 CFR) Part 261 identifies compounds for which specific hazardous wastes, from specific and nonspecific sources, are listed (U.S. EPA 1995). Appendix VIII of 40 CFR Part 261 identifies acute hazardous wastes and toxic hazardous wastes associated with commercial chemical products, manufacturing chemical intermediates, and off-specification commercial chemical products (U.S. EPA 1995). This column lists hazardous waste codes for the associated compounds. This list is provided for reference purposes only, because it is commonly cited by other U.S. EPA combustion risk assessment documents as an original source of the product of incomplete combustion (PIC) lists. An explanation of the reasons for including a COPC on this list is beyond the scope of this guidance.

A1.4 COLUMN 4: CHEMICAL-SPECIFIC DATA AVAILABLE

This column lists those compounds for which the following are available (as presented in Appendix A-2): (1) chemical-specific physical and chemical information, and (2) chemical-specific fate-and-transport information.

A1.5 COLUMN 5: PICS RECOMMENDED BY U.S. EPA (1994a) FOR SCREENING LEVEL RISK ASSESSMENTS

Compounds in this column marked with an "X" in the appropriate cells identified by U.S. EPA (1994a) as PICs to be included in screening level risk assessments. U.S. EPA (1994a) does not describe the basis or references for the inclusion of these PICs in screening level risk assessments. More information regarding some of these compounds is presented in Chapter 2.

A1.6 COLUMN 6: PICS IDENTIFIED IN COMBUSTION UNIT EMISSIONS (U.S. EPA 1993)

Compounds in this column marked with an "X" in the appropriate cells are identified in U.S. EPA (1993) as PICs. The source documents for these tables cited by U.S. EPA (1993) are described in the following subsections. These references have been cited by this and other U.S. EPA reference documents as "sources" of information regarding PIC emissions from hazardous waste combustion units. This document—U.S. EPA (1993)—has, in turn, been cited by later guidance documents as a "source" of information regarding PIC emissions from hazardous waste combustion units. However, as is indicated by the listing of the references from Dempsey and Oppelt (1993) (which is a summary of existing information), many of the reference documents appear to simply cite additional "sources" of information. The original research and sampling data regarding PIC emissions have not yet been identified but, based on a preliminary review of the information below, the sources of the "original" information cited by all of the most common reference documents may be limited and may have been published over 15 years ago.

A1.6.1 Demsey and Oppelt (1993)

The sections of Demsey and Oppelt (1993) regarding PICs from hazardous waste combustion facilities ("Combustion Byproduct Emissions" and "Table XVII: Organics that Could Potentially be Emitted from Devices Burning Hazardous Waste") cite the following references:

- U.S. EPA (1989b) does not include a list of PICs from combustion sources. U.S. EPA (1989b) discussed ways of ensuring that PIC emissions do not pose an unacceptable risk to human health and the environment. Stack gas carbon monoxide (CO) concentration is a good indicator of combustion efficiency; therefore, controlling CO is a prudent and reasonable approach to minimizing the potential risk from PICs. The destruction and removal efficiency (DRE) standard of 40 CFR Part 264.242(a) limits stack emissions of principal organic hazardous constituents (POHC) to 0.01 percent (or 0.0001 percent for dioxin-containing waste) of the quantity of POHC in the waste. This standard, however, does not impose a limit on PICs. Therefore, a limit of 100 parts per million by volume (ppmv) (Tier I) was imposed, below which PIC emissions do not pose unacceptable risks to human health. The proposed rule allows a waiver to the 100-ppmv CO limit, by (1) restricting total hydrocarbon (THC) emissions to 20 ppmv (Tier II), or (2) showing that THC emissions do not pose an unacceptable risk by using prescribed risk assessment procedures.

  The above limitations were also provided in the Federal Register, dated January 23, 1981 (U.S. EPA 1981) and April 27, 1990 (U.S. EPA 1990b)

- U.S. EPA (1981) does not contain any information regarding PICs not contained in U.S. EPA (1989b). There is no discussion of "risk" in this document. Although the notice deals with permitting standards, there is no risk-based approach, and it appears to be an entirely technical discussion. Specifically, it deals with updated material for specific parts of 40 CFR.

  - 40 CFR Part 122 (Incinerator Facility Permits)
  - 40 CFR Part 264 (General Standards for Hazardous Waste Incineration)
  - 40 CFR Part 265 (Interim Status Standards for Hazardous Waste Incineration)

Standards are technology-based, not risk-based.

- U.S. EPA (1990a) describes amendments to the hazardous waste incinerator regulations for the following purpose:

  > Improve control of toxic metal emissions, HCl emissions, and residual organic emissions; amend the definitions of incinerators and industrial furnaces; propose definitions for plasma arc incinerators and infrared incinerators; propose to regulate carbon regeneration units as thermal treatment devices; and make a number of minor revisions to permitting procedures.

  U.S. EPA (1990a) also states the following:

  > The database on PIC emissions is limited therefore, the risk assessments may under-estimate risk. The assessments consider only the organic compounds that have been actually identified and quantified. Zero to 60 percent of total unburned hydrocarbon emissions have been chemically identified at any particular facility. Thus, the bulk of the hydrocarbon emissions have not been considered in those risk assessments. Although many of the unidentified, unquantified organic compounds may be non-toxic, some fraction of the organic emissions is undoubtedly toxic. . . .data on typical PIC emissions from hazardous waste combustion sources were compiled and assessed in recent EPA studies. These studies identified 37 individual compounds in the stack gas of the eight full-scale hazardous waste incinerators tested, out of which 17 were volatile compounds and 20 semivolatile compounds. Eight volatile compounds (benzene, toluene, chloroform, trichloroethylene, carbon tetrachloride, tetrachloroethylene, chlorobenzene, and methylene chloride), and one semivolatile compound (naphthalene) were identified most frequently in more than 50 percent of the tests. Some of these compounds are carcinogenic.

  The sources for these statements appear to be Wallace and others (1986) and Trenholm and Lee (1986).

  Trenolm and Lee (1986), prepared by Andrew R. Trenholm of Midwest Research Institute and C.C. Lee at the U.S. EPA Hazardous Waste Engineering Research Laboratory, discussed that emissions from incinerators are only characterized for constituents listed in Appendix VIII. However, constituents not listed in Appendix VIII are also emitted from the stacks.

  Data was obtained from HWERL-sponsored tests at eight hazardous waste incinerators, nine boilers that co-fired hazardous wastes, and five mineral processing kilns that fired hazardous wastes as fuel. In addition, SVOC emissions data for two municipal solid waste incinerators and seven coal-fired power plants were also reviewed. The common PICs are presented in the following table:

Volatile PICs Most Frequently Present in Stack Gases	
VOCs	**SVOCs**
Benzene	Naphthalene
Toluene	Phenol
Carbon Tetrachloride	Bis(2-ethylhexyl)phthalate
Chloroform	Diethylphthalate
Methylene Chloride	Butylbenzylphthalate
Trichloroethylene	Dibutylphathlate
Tetrachloroethylene	
1,1,1-Trichloroethane	
Chlorobenzene	

Tests were conducted for three incinerator runs to search for constituents not listed in Appendix VIII . These constituents include:

Non-Appendix VIII Constituents Present in Highest Concentrations in Stack Gases	
Acetone	Ethylbenzaldehyde
Ethylbenzene	Ethylbenzoic acid
Acetophenone	Ethylphenol
Benzaldehyde	Ethylphenyl-ethanone
Benzenedicarboxaldehyde	Ethynylbenzene
Benzoic acid	Phenylacetylene
Chlorocyclohexanol	1,1'-(1,4-phenylene)bisethanone
Cyclohexane	Phenylpropenol
Cyclohexanol	Propenylmethylbenzene
Cyclohexene	Tetramethyloxirane
Dioctyl adipate	Trimethylhexane
Ethenyl ethylbenzene	

Emission rates of compounds not in the waste feed were also provided.

- U.S. EPA (1985) does not include a list of PICs from combustion sources. U.S. EPA (1985) discussed views and reviews by the Environmental Effects, Transport, and Fate Committee of the Science Advisory Board of issues related to the environmental impacts of the incineration of liquid hazardous wastes at sea and on land. Several issues were

addressed, including issues concerning the combustion and incineration of hazardous waste. Major findings of the committee were as follows:

- Fugitive emissions and spills may release as much or more material to the environment than the direct emissions from waste incineration processes.

- Numerous PICs are formed during combustion processes. However, only a fraction of them are identified or detected. It is possible that the aggregate of all compound emissions that are not categorized as other POHCs or PICs can be more toxic and pose greater risks than those listed. Although 99.99 percent DRE has been claimed, if the unburned or undetected hydrocarbon output is included, the DRE may actually be less than 99.99 percent. Therefore, the concept of destruction efficiency used by EPA was found to be incomplete and not useful for subsequent exposure assessments. All emissions and effluents must be identified and quantified, including their physical form and characteristics.

- Local site-specific conditions must be used in characterizing exposure to receptors from waste incinerator emissions.

- The evaluation of exposure durations and concentrations should be based on a detailed assessment of transport processes and the habits of the exposed organisms. The role of food chains needs particular attention.

- At a minimum, the toxicities of representative emissions and effluents from incinerators should be tested on sensitive life stages of representative aquatic and terrestrial vertebrates, invertebrates, and plants of ecological importance.

• U.S. EPA (1990b) does not include a list of PICs from combustion sources. It was prepared by the PIC subcommittee of the Science Advisory Board to review the OSW proposal to control emissions of PICs from hazardous waste incinerators by instituting process controls that are based on CO and THC emission concentrations. U.S. EPA risk assessments indicate that emissions of PICs at currently measured levels are not likely to produce unacceptable risks. However, because the current DRE standard applies only to designated POHCs, 99.99 percent DRE does not preclude the possibility that emission of PICs could present significant risk. The following summarizes the major findings of the subcommittee review.

  - The concept of using CO and THC as guidance for incinerator operational control is reasonable.

  - At low CO levels, CO correlates well with THC; therefore, limiting CO in order to ensure high combustion efficiency and low THC levels is reasonable. At high CO concentrations, CO and THC do not correlate well; therefore, relying solely on the controlling of CO may not provide a reasonable control for THC. Continuous emissions monitoring of THC is preferred. Quantification of PICs alone is not practical with the sampling techniques that are available, primarily because PICs are normally emitted in the range of parts per billion (ppb) to parts per trillion (ppt).

- A 100-ppmv limit for CO is reasonable. However, supporting documentation does not demonstrate that a CO concentration of 100 ppmv is better than 50 ppmv or 150 ppmv.

- Continuous emissions monitoring of THC with a cold system appears to be practical for routine operations. However, a hot transfer line produces better analysis of THC concentrations and detection of a larger fraction of the THCs emitted.

- The database characterizing PICs in emissions would not allow a correlation to be established with CO or THC levels for various combustion devices and conditions. Limited data introduces large uncertainties into U.S. EPA's risk assessment. Therefore, U.S. EPA's site-specific risk assessment process is limited in its usefulness in establishing acceptable THC levels. However, the risk assessment procedures are risk-based.

• U.S. EPA (1987) is a report prepared by Andrew R. Trenholm, Acurex Corporation, California, and staff members from the U.S. EPA Hazardous Waste Engineering Research Laboratory in Cincinnati, Ohio. The paper discussed the lack of information on total emissions from combustion of hazardous wastes, particularly under conditions of less than optimal performance. The focus issue was whether additional constituents that are listed in Appendix VIII or not listed in Appendix VIII which were not identified in early tests might be emitted from hazardous waste combustion units. To address this issue and related issues, U.S. EPA initiated this project to qualitatively and quantitatively study the characteristics of all possible effluents, under steady-state and transient conditions. The following summarizes the major findings:

  - THC emissions detected as specific compounds ranged from 50 to 67 percent for five runs and were 91 percent for one run. The fraction of THC not detected is most likely explained by uncertainty in the measurements or other analytical problems.

  - Methane accounted for the largest fraction of THC.

  - Oxygenated aliphatic compounds made up the largest class of compounds among the SVOCs, both in total mass and number of compounds.

  - Transient upsets did not cause significant increases in the concentration of SVOCs or most VOCs. Three VOCs that were increased were methane, methylene chloride, and benzene.

  - Particulate and HCl emissions did not change between the steady-state and transient test runs.

• Duval and Rubey (1976) was prepared by D.S. Duval and W.A. Rubey of the University of Dayton Research Institute, Ohio. The objective of the study was to provide data from which requirements can be assigned for the thermal disposal of kepone. This report was primarily concerned with the high-temperature destruction of kepone, with DDT and Mirex used as comparative Analog. Laboratory tests were conducted to establish

destruction temperature characteristics of the vaporized pesticides at preselected residence times. The following summarizes the major findings.

- Kepone was essentially destroyed at a 1-second residence time and a temperature range of 500°C to 700°C, depending on the pesticide.

- Major decomposition products detected were hexachlorocyclopentadiene and hexachlorobenzene for both kepone and Mirex. These products were formed in different thermal regions.

- The study demonstrated that the chemical nature of the effluent products depends on the temperature and residence time that the basic molecule experiences.

- Duval and Rubey (1977) discusses the experimental destruction temperature and residence time relationships for various PCB compounds and mixtures of PCBs. The document states that "upon thermal stressing in air, PCBs decomposes to low-molecular-weight products." However, the document does not identify any of these low-molecular-weight products. In fact, the document states directly that the products were not identified in the study. It further recommends that additional research be conducted on the "degradation products and effluents."

- Dellinger, Torres, Rubey, Hall, and Graham (1984) was prepared by Barry Dellinger and others of the University of Dayton, Ohio. This paper presented the gas-phase thermal stability method under controlled laboratory conditions to rank the incinerability of compounds. The objective of this study was to determine the gas-phase thermal decomposition properties of 20 hazardous organic compounds.

  The compounds were selected on the basis of (1) frequency of occurrence in hazardous waste samples, (2) apparent prevalence in stack effluents, and (3) representativeness of the spectrum of hazardous waste organic waste materials. The following summarizes the major findings.

  - Gas-phase thermal stability method is a more effective means of ranking the incinerability of hazardous compounds in a waste.

  - Numerous PICs were formed during the thermal decomposition of most of the compounds tested. However, PICs were not identified.

  - Destruction efficiency of 99.99 percent is achieved at 2 seconds mean residence time in flowing air at 600°C to 950 °C.

  - No single physical or chemical property describes the ranking scheme for incinerability.

- Dellinger, Hall, Graham, Mazer, Rubey, and Malanchuk (1986) was prepared by Barry Dellinger, B. Douglas, L. Hall, John L. Graham, Sueann L. Mazer, and Wayne A. Rubey of the University of Dayton Research Institute, Dayton, Ohio, and Myron Malanchuk of U.S. EPA, Cincinnati, Ohio. The paper discussed the development of an incineration

model based on laboratory studies conducted by using the nonflame mode of hazardous waste thermal decomposition. The results of these studies were compared to the flame-mode studies and field tests to evaluate the incineration model proposed. The model was based on the premise that incinerators do not operate continuously at optimum conditions. As a result, 1 percent or more of the feed and its flame treatment products must undergo further decomposition in the nonflame region to meet the DRE criterion of greater than 99.99 percent.

In the past, several methods were used to rank the incinerability of compounds. Nonflame studies, however, indicated that tests on compounds conducted at low oxygen concentrations provided a better correlation with field tests to determine the relative incinerability of compounds. Four experimental studies were conducted to develop and expand the database on POHCs and PICs.

Studies were conducted on individual compounds to evaluate degradation compounds and PICs from the original parent compound. The thermal degradation of 2,3',4,4',5-PCB was studied under four reaction atmospheres (at varying levels of oxygen) at a constant gas phase residence time of 2.0 seconds. Tests were conducted at temperatures ranging from 500°C to 1,000°C. Tests indicated that the yield of combustion products decreased with increased oxygen levels. Numerous major degradation products were identified from the thermal degradation of 2,3',4,4',5-PCB, including:

- Penta-, tetra-, and trichlorodibenzofurans
- Tetra- and trichlorobiphenyls
- Tri- and dichlorobenzene
- Tetra- and trichloronaphthalene
- Tri- and dichlorochlorophenylethlyene
- Tetrachlorobiphenylenes
- C_9H_8OCl
- $C_{10}H_3Cl_3$

Thermal decomposition of chloroform was studied. Numerous decomposition products were identified, including:

- CCl_4
- $C_2H_4Cl_2$
- C_2HCl_3
- C_2HCl_5
- C_2Cl_2
- C_2Cl_4
- C_3Cl_4
- C_4Cl_6

Thermal decomposition of polychlorinated phenols was studied in nitrogen (N_2) and oxygen atmospheres because of the potential formation of polychlorinated dibenzodioxins. Pentachlorophenol (PCP) thermal decomposition was studied. Numerous decomposition products of PCP were identified in N_2 and/or air atmospheres, including:

- Dichlorobutadiyne (in N_2)
- Tetrachloroethylene (in air)
- Tetrachloropropyne (in air)
- Trichlorofuran (in air)
- Tetrachlorofuran (in air)
- Trichlorobenzene (in N_2 and air)
- Tetrachlorobenzene (in N_2 and air)
- Pentachlorobenzene (in N_2 and air)
- Hexachlorobenzene (in N_2)
- Octachlorostyrene (in N_2)
- Hexachlorodihydronaphthalene (in N_2 and air)

The paper concluded that PICs in the air atmosphere may have formed directly from the parent material, whereas, in the nitrogen atmosphere, the principal PICs may have evolved from the thermal decomposition of other PICs.

- Kramlich, Seeker, and Heap (1984) does not include a list of PICs from combustion sources. It was prepared by J.C. Kramlich, W.R. Seeker, and M.P. Heap of Energy and Environmental Research Corporation, California; and C.C. Lee of the Industrial Waste Combustion Group, U.S. EPA. This paper presented a research program to study the flame-mode incineration of hazardous waste liquids in laboratory scale reactors. The objective of this study was to supply the flame-mode data that will be used in evaluating the applicability of various approaches to ranking the ease of incinerability.

  Five compounds were tested—chloroform, 1,1-dichloroethane, benzene, acrylonitrile, and chlorobenzene—because (1) their range of incinerabilities is broad, and (2) they are representative of liquid hazardous wastes. The following summarizes the findings.

  - The flame section of the incinerator destroys greater than 99.995 percent of the wastes.
  - The post-flame region destroys the remainder of the wastes.
  - The destruction efficiency is reduced because of flame-related failures.
  - Incinerability ranking depends on actual failure condition.
  - No incinerability ranking system completely predicts the destruction efficiency of the compounds tested for all failure conditions.

- Trenholm and Hathaway (1984) was prepared by Andrew Trenholm and Roger Hathaway of Midwest Research Institute (MRI) in Missouri, and Don Oberacker, U.S. EPA, Cincinnati, Ohio. PICs were defined as any Appendix VIII hazardous organic constituent detected in the stack gas but not present in the waste feed at a concentration of 100 micrograms per gram or higher. Benzene and chloroform were the most commonly found PICs. PIC emissions were comparable to POHC emissions in concentration and total mass output. This document discussed PIC formation mechanisms and criteria for PIC formations.

MRI conducted a series of tests at eight operating hazardous waste incineration facilities and analyzed the collected samples for PICs. These tests were conducted as part of the technical support of U.S. EPA's preparation of a regulatory impact analysis for hazardous waste incinerators. Each incinerator had a liquid injection burner, and some facilities also included a rotary kiln or hearth. Three incinerators had no air pollution control devices. The remaining five had wet scrubbers for HCl control, and four of these had other particulate control devices. Twenty-nine compounds were classified as PICs from the eight incinerator tests and are presented in Table A1.6-1. In general, PIC concentrations were slightly higher than POHC concentrations, although this ratio varied from site to site. PIC output rate very rarely exceeded 0.01 percent of the POHC input rate. The document stated that the measurement of Appendix VIII compounds at low concentrations in the waste feed, auxiliary fuel, and inflow streams to control systems is often necessary to explain the presence of PICs.

- Olexsey, Huffman, and Evans (1985) was prepared by Robert A. Olexsey and others of the U.S. EPA Hazardous Waste Engineering Research Laboratory in Cincinnati, Ohio. This document discussed PIC generation mechanisms and criteria for PIC formations. The paper provided data on emissions of PICs during full-scale tests conducted on incinerators and boilers burning hazardous waste (Trenholm and others 1984; Castaldini and others 1984). The documents referenced by this paper summarized a series of full-scale tests conducted on seven incinerators and five boilers conducted by U.S. EPA to support its regulatory development for incinerators and boilers. Commonly found PICs identified in these tests are presented in Tables A1.6-2 and A1.6-3.

- For incinerators, ratios of PIC emissions to POHC input ranged from 0.00007 to 0.0028 percent; and ratios of PIC emissions to POHC emissions ranged from 0.01 to 3.89. For boilers, ratios of PIC emissions to POHC input ranged from 0.0032 to 0.3987 percent, and ratios of PIC emissions to POHC emissions ranged from 5.44 to 22.5. These data indicated that PIC emissions were higher for boilers than for incinerators; that is, PIC emissions were reduced with increased POHC DRE which is higher for incinerators. The document proposed seven methods to control PICs and recommended further research on PIC generation mechanisms and control technologies.
- Trenholm, Kapella, and Hinshaw (1992) was prepared by Andrew R. Trenholm and David W. Kapella of MRI in North Carolina and Gary D. Hinshaw of MRI in Missouri. The paper discusses the following issues regarding emissions from incinerators that burn hazardous waste: (1) emissions of specific constituents presented in Appendix VIII, (2) emissions of specific compounds or types of compounds, and (3) data on the size and molecular weight of compounds emitted. The following were among the major issues discussed.

    - PICs were studied through U.S. EPA-sponsored tests at eight incinerators, nine industrial boilers, and five mineral processing kilns. The study was limited to compounds presented in Appendix VIII. In all, 52 organic compounds (32 VOCs and 20 SVOCs) were identified. The VOC concentrations were significantly higher than the SVOC concentrations. PICs listed in this paper included benzene, toluene, carbon tetrachloride, trichloromethane, dichloromethane, trichloroethene, tetrachloroethene, 1,1,1-trichloroethane, cholorobenzene, naphthalene, and phenol.

TABLE A1.6-1

PICS IDENTIFIED BY TRENHOLM AND HATHAWAY (1984)

PICs Found In Stack Effluents			
PIC	Number of Facilities	Low Concentration (ng/L)	High Concentration (ng/L)
Benzene	6	12	670
Chloroform	5	1	1,330
Bromodichloromethane	4	3	32
Dibromochloromethane	4	1	12
Naphthalene	3	5	100
Bromoform	3	0.2	24
Chlorobenzene	3	1	10
Tetrachloroethylene	3	0.1	2.5
1,1,1,-Trichloroethane	3	0.1	1.5
Toluene	2	2	75
o-Nitrophenol	2	2	50
Methylene chloride	2	2	27
Phenol	2	4	22
2,4,6-Trichlorophenol	1	110	110
Carbon disulfide	1	32	32
o-Chlorophenol	1	22	22
2,4-Dimethylphenol	1	21	21
Methylene bromide	1	18	18
Bromochloromethane	1	14	14
Trichlorobenzene	1	7	7
Hexachlorobenzene	1	7	7
Diethyl phthalate	1	7	7
Pentachlorophenol	1	6	6
Dichlorobenzene	1	4	4
Chloromethane	1	3	3
Methyl ethyl ketone	1	3	3
Bromomethane	1	1	1
Pyrene	1	1	1
Fluoranthene	1	1	1

Notes:

ng/L = Nanograms per liter
PIC = Product of incomplete combustion

TABLE A1.6-2

VOLATILE PICS MOST FREQUENTLY IDENTIFIED IN BOILER EMISSIONS (OLEXSY, HUFFMAN, AND EVANS 1985)

PIC	Number of Facilities	Low Concentration (ng/L)	High Concentration (ng/L)
Chloroform	5	4.2	1,900
Tetrachloroethylene	5	0.3	760
Chloromethane	4	4.6	410
Methylene chloride	4	83	2,000
Benzene	3	9.4	270
1,1,1-Trichloroethane	3	5.9	270
1,2-Dichloroethane	3	1.3	1,200

Notes:
ng/L = Nanograms per liter
PIC = Product of incomplete combustion

TABLE A1.6-3

VOLATILE PICS MOST FREQUENTLY IDENTIFIED IN INCINERATOR EMISSIONS (OLEXSY, HUFFMAN, AND EVANS 1985)

PIC	Number of Facilities	Low Concentration (ng/L)	High Concentration (ng/L)
Benzene	6	12	670
Chloroform	5	1	1,330
Tetrachloroethylene	3	0.1	2.5
1,1,1-Trichloroethane	3	0.1	1.5
Toluene	2	2	75
Methylene chloride	2	2	27

Notes:

ng/L = Nanograms per liter
PIC = Product of incomplete combustion

- From the U.S. EPA-sponsored tests, (1) volatile compounds listed in Appendix VIII identified were only a fraction—sometimes about one-half—of the total organic compounds identified, and (2) semivolatile compounds not listed in Appendix VIII identified were three to 30 times the quantity of organic compounds listed in Appendix VIII . Table A1.6-4 lists the compounds identified by the U.S. EPA-sponsored tests.

- A study of hazardous waste incinerator stack effluent was conducted to characterize the types of compounds emitted. Twenty-nine compounds were identified at a concentration range of 0.1 to 980 nanograms per liter. Methane, chloromethane, and chloroform accounted for more than one-half of the total mass of VOCs detected. Other than methane, oxygenated aliphatic hydrocarbons formed the highest fraction of the total emissions.

- Based on the incinerator stack effluent study, it was found that as combustion conditions deteriorate, increases in mass emissions are first noted with VOCs. Emissions of these compounds, most notably C1 to C3 compounds, increase proportionately more than larger compounds. For larger compounds, available data indicate that emission increases are more likely to be aromatic compounds.

A1.6.3 CARB (1990b)

CARB prepared "Technical Support Document of Proposed Dioxins Control Measures for Medical Waste Incinerators" to meet the requirements of California Health and Safety Code Section 39666 that a needs report be prepared for proposed rules. The report presents a proposed airborne toxic control measure for dioxin emissions from medical waste-burning facilities. The report concentrates on dioxin, furan, and cadmium emissions, although other pollutants detected during the tests are listed. Table A1.6-5 lists these pollutants.

A1.6.4 CARB (1991)

CARB prepared "Air Pollution Control at Resource Recovery Facilities 1991 Update" to update information presented in its 1984 report, entitled "Air Pollution Control at Resource Recovery Facilities." Specifically, the document updates available guidelines concerning incinerator technology, emissions control technology, and emission limits for municipal waste, hospital waste, biomass, tire, manure, landfill and digester gas, and sewer sludge incinerators. The document states that its guidelines represent levels that have been achieved by existing facilities.

In addition, the document summarizes the ultimate analysis of waste types undergoing treatment in the facilities described above. An appendix summarizes stack gas analysis data for numerous operating facilities. Pollutants identified in the analyses are summarized in Table A1.6-6.

TABLE A1.6-4

MOST FREQUENTLY IDENTIFIED PICS (TRENHOLM, KAPELLA, AND HINSHAW 1992)

Appendix VIII Volatile Organic Compounds	Appendix VIII Semivolatile Organic Compounds	Compounds Not Listed in Appendix VIII
1,1,1-Trichloroethane	Bis(2-Ethylhexyl)phthalate	1,1'-(1,4-Phenylene)bisethanone
Benzene	Butylbenzylphthalate	Acetone
Carbon tetrachloride	Dibutylphtahlate	Acetophenone
Chlorobenzene	Diethylphthalate	Benzaldehyde
Chloroform	Naphthalene	Benzenedicarboxaldehyde
Methylene chloride	Phenol	Benzoic acid
Tetrachloroethylene		Cyclohexanol
Toluene		Chlorocyclohexanol
Trichloroethylene		Cyclohexane
		Ethylbenzene
		Ethylbenzoic acid
		Ethylphenol
		Ethylphenyl-ethanone
		Ethynylbenzene
		Phenylpropenol
		Propenylmethylbenzene
		Tetramethyloxirane
		Trimethylhexane

TABLE A1.6-5

COPCS IDENTIFIED BY CARB (1990b)

COPC		
Ammonia	1,2-Dibromoethane	Nickel
Arsenic	Dichloroethane	Nitrogen oxides
Benzene	Dichloromethane	PM
Bromodichloromethane	1,2-Dichloropropane	PAHs
Cadmium	Ethylbenzene	Sulfur dioxide
Carbon dioxide	Freon	Tetrachloroethene
Carbon monoxide	Hydrocarbon, total	Tetratrichloromethylene
Carbon tetrachloride	Hydrogen chloride	Toluene
Chlorobenzenes	Hydrogen fluoride	Tribromomethane
Chlorodibromomethane	Iron	Trichlorethane
Chloroform	Lead	1,1,1-Trichloroethane
Chlorophenols	Manganese	Trichloroethylene
Chromium, hexavalent	Mercury	Trichlorotrifluroethane
Chromium, total	Mesitylene	Vinyl chloride
Copper	Methyl isobutyl ketone	Xylenes
Cumene	Napthalene	Zinc

Notes:

PAH = Polynuclear aromatic hydrocarbons
PM = Particulate matter

TABLE A1.6-6

STACK GAS ANALYSIS DATA
(CARB 1991)

(Page 1 of 2)

Pollutant	Incinerator Type [a]						
	Municipal Waste (5)	Hospital Waste (7)	Biomass (4)	Manure (1)	Tire (1)	Landfill Gas (20)	Sewage Sludge and Digester Gas (5)
Nitrogen oxides	✔	✔	✔	✔	✔	✔	✔
Sulfur oxides	✔	✔	ND	✔	✔	✔	✔
Particulate matter	✔	✔	✔	✔	✔	✔	✔
Carbon monoxide	✔	✔	✔	✔	✔	✔	✔
Total hydrocarbons	✔	✔	✔	✔	✔	✔	✔
Hydrogen chloride	✔	✔	NA	NA	✔	NA	NA
Hydrogen fluoride	✔	NA	NA	NA	NA	NA	NA
Amonnia	NA	NA	✔	NA	✔	NA	NA
Carbon dioxide	✔	✔	✔	✔	✔	NA	✔
Oxygen	✔	✔	✔	✔	✔	NA	✔
Arsenic	✔	✔	✔	NA	✔	✔	✔
Beryllium	✔	NA	NA	NA	✔	✔ [b]	✔
Cadmium	✔	✔	✔	NA	ND	✔ [b]	✔
Chromium (total)	✔	✔	✔	NA	✔	✔	✔
Chromium (hexavalent)	ND	✔	NA	NA	✔	NA	NA
Copper	✔	NA	NA	NA	NA	✔	NA
Mercury	✔	✔	NA	NA	ND	✔	✔
Iron	NA	NA	✔	NA	NA	NA	NA
Manganese	NA	NA	✔	NA	NA	NA	NA
Nickel	✔	✔	✔	NA	ND	✔	✔
Lead	✔	✔	✔	NA	ND	✔	✔
Zinc	NA	NA	NA	NA	NA	✔	NA
Polyaromatic hydrocarbons [b]	✔	NA	✔	NA	✔	NA	NA
Polychlorinated biphenyls [b]	✔	ND	✔	NA	✔	NA	NA
CP [b]	✔	NA	✔	NA	✔	NA	NA
CB [b]	✔	NA	✔	NA	✔	NA	NA
Benzene	✔	✔	✔	NA	NA	NA	NA
Polychlorinated dibenzo(p) dioxins [b]	✔	✔	✔	NA	✔	NA	NA
Polychlorinated dibenzofurans [b]	✔	✔	✔	NA	✔	NA	NA
2,3,7,8-Tetrachloro dibenzo(p)dioxin equivalents [b]	✔	✔	✔	NA	✔	NA	✔

TABLE A1.6-6

STACK GAS ANALYSIS DATA
(CARB 1991)

(Page 2 of 2)

Notes:

✔	=	Detected in at least one emission test
ND	=	Not detected in any emission test
NA	=	No analysis

[a] Number in parentheses indicates the number of facilities for which data were tabulated.

[b] Isomers and/or homologues that were not detected were added to total values at one-half the detection limit; pollutant may not have actually been detected.

A1.6.5 U.S. EPA (1988)

This document, referenced by some documents as a 1989 document, was prepared in 1988.

U.S. EPA prepared "Hospital Waste Combustion Study: Data Gathering Phase" to assemble available information on hospital waste combustion so that U.S. EPA can evaluate whether airborne pollutant emissions from hospital waste combustion should be regulated. While preparing this document, U.S. EPA reviewed the pertinent literature to determine which studies would be helpful in completing the database on toxic emissions from medical waste incinerators. The report clearly addresses only those pollutants for which emissions data were found. The data reviewed were mostly for larger, controlled air incinerators; and the more commonly used retort incinerators were not evaluated.

The study identified several categories of pollutants that were measured in stack gases; these are discussed in the following paragraphs.

Where evaluated, acid gases were detected in stack gases. For example, HCl was detected in 24 of 28 tests; HCl concentration not recorded in the remaining four tests.

Particulate matter (PM) was detected in all stack tests for 30 facilities at concentrations ranging from 0.001 grains per dry standard cubic foot (gr/dscf), at a facility with PM add-on control devices, to 0.22 gr/dscf at facilities without such control devices.

Trace metals were detected in stack tests for three medical waste incineration facilities. Metals detected include arsenic, cadmium, chromium, iron, manganese, nickel, and lead. The document also states that fine-particle enrichment processes could lead to emissions of molybdenum, tin, selenium, vanadium, and zinc. However, test results for these trace metals are not presented.

With respect to organic emissions, dioxins and furans were detected in emissions from three facilities, both with and without pollution control devices. Other organic emissions detected in stack tests cited in this report include CO, THC, trichlorotrifluoroethane, tetrachloromethane, tetrachloroethene, and trichloroethylene.

In a stack testing conducted on three Canadian biomedical waste incinerators, PCBs and PAHs were either not detected (one facility) or not analyzed (two facilities).

A1.6.6 CARB (1996)

In May 1996, CARB prepared "Proposed Amendments to the Emission Inventory Criteria and Guidelines Report Published in Accordance with the Air Toxics ‘Hot Spots’ Information and Assessment Act of 1987." The purpose of the report is to present the basis of CARB’s recommended amendments to the Air Toxics Hot Spots Program. The report states that California Health and Safety Code (HSC) 44321 requires CARB to compile the list of toxic substances that must be monitored from "designated reference lists of substances." Therefore, the document is not a primary source of toxics emission information. The primary sources of information are mandated by California HSC 44321, as follows:

- California HSC 44321(a): National Toxicology Program, International Agency for Research on Cancer
- California HSC 44321(b): Governor’s List of Carcinogens and Reproductive Toxicants

- California HSC 44321(c): CARB
- California HSC 44321(d): Hazard Evaluation System and Information Service
- California HSC 44321(e): U.S. EPA
- California HSC 44321(f): California HSC

The lists of toxic substances presented in the document are not restricted to incinerator facilities, but apply to any facility discharging airborne pollutants to the atmosphere. The document also removes numerous substances, primarily medicinal compounds, from lists of toxic chemicals that must always be evaluated, and places them on lists of toxic compounds that require evaluation only if a facility manufactures that substance.

A1.7 COLUMN 7: U.S. EPA-RECOMMENDED AND POTENTIAL PICS (1994a; 1994b)

Compounds marked with an "X" in the appropriate cells are identified in U.S. EPA (1994a and 1994b). Based on information presented in U.S. EPA (1994b), these tables were developed from available U.S. EPA data and from lists of toxic compounds from various U.S. EPA programs. Because the source lists were not developed as lists of toxic PICs, U.S. EPA deleted compounds that were not appropriate (U.S. EPA 1994b). U.S. EPA acknowledged the importance of using focused studies to develop a PIC list that is (1) appropriately protective of the environment, and (2) not excessively burdensome on the regulated community. Nevertheless, Tables 1 and 2 in U.S. EPA (1994b) were compiled as draft lists for use during the interim period. Tables in U.S. EPA (1994b) were to be revised as additional PIC data were collected. U.S. EPA Permits and State Program Division is currently updating these tables; however, a target completion date is not available. Tables 1 and 2 are based on the following (U.S. EPA 1994b):

- Hazardous waste constituent list in 40 CFR Part 261, Appendix VIII
- hazardous air pollutants (HAP) list
- Office of Research and Development list of organic compounds found in combustion devices developed for U.S. EPA (1993)

The following compounds were deleted from this list:

- Pesticide compounds not likely to be a PIC
- Federal Drug Administration-regulated drugs
- Carcinogenic sugar substitutes
- Compounds without chemical-specific listings (for example, "coal tar")
- Compounds without U.S. EPA-established sampling and analysis methods
- Metallic compounds (because of difficulty in analyzing the specific compounds; metals are still included in elemental totals)

- Compounds with low octanol-water partition coefficients and no inhalation toxicity data
- Compounds with low toxicity values
- Naturally-occurring plant toxins

Specific compounds were retained on Tables 1 and 2 on the following basis:

- Pesticides with a molecular structure simple enough to be of concern as a PIC
- Compounds with very high octanol-water partition coefficients

A1.8 COLUMN 8: PICS ACTUALLY DETECTED IN STACK EMISSIONS

Compounds marked by an "X" in the appropriate cells are PICs that have actually been detected in stack emissions. U.S. EPA compiled this list by evaluating the studies highlighted in Section A1.6.

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APPENDIX A-2

COMPOUND SPECIFIC PARAMETER VALUES

Screening Level Ecological Risk Assessment Protocol

August 1999

APPENDIX A-2

TABLE OF CONTENTS

APPENDIX A-2

LIST OF VARIABLES AND COMPOUND-SPECIFIC PARAMETERS

ρ_{air}	=	Density of air (g/cm^3)
ρ_{forage}	=	Density of forage (g/cm^3)
Ba_{beef}	=	Biotransfer factor in beef (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
$Ba_{chicken}$	=	Biotransfer factor in chicken (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
Ba_{egg}	=	Biotransfer factor in eggs (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
Ba_{milk}	=	Biotransfer factor in milk (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
Ba_{pork}	=	Biotransfer factor in pork (mg COPC/kg FW tissue)/(mg COPC/day) OR (day/kg FW tissue)
BAF_{fish}	=	Bioaccumulation factor in fish (mg COPC/kg FW tissue)/(mg COPC/L total water column) OR (L water/kg FW tissue)
BCF_{fish}	=	Bioconcentration factor in fish (L/kg FW OR unitless)
Br_{ag}	=	Plant-soil bioconcentration factor in aboveground produce (µg COPC/g DW plant)/(µg COPC/g DW soil)—unitless
$Br_{forage/silage}$	=	Plant-soil bioconcentration factor in forage and silage (µg COPC/g DW plant)/(µg COPC/g DW soil)—unitless
Br_{grain}	=	Plant-soil bioconcentration factor in grain (µg COPC/g DW grain)/(µg COPC/g DW soil)—unitless
$Br_{rootveg}$	=	Plant-soil bioconcentration factor for belowground produce (µg COPC/g DW plant)/(µg COPC/g DW soil)—unitless
$BSAF_{fish}$	=	Biota-sediment accumulation factor in fish (mg COPC/kg lipid tissue)/(mg COPC/kg sediment)—unitless
B_{vol}	=	Volumetric air-to-leaf biotransfer factor in leaf (µg COPC/L FW plant)/(µg COPC/L air)—unitless
Bv_{ag}	=	COPC air-to-plant biotransfer factor for aboveground produce (µg COPC/g DW plant)/(µg COPC/g air)—unitless
$Bv_{forage/silage}$	=	Air-to-plant biotransfer factor in forage and silage (µg COPC/g DW plant)/(µg COPC/g air)—unitless
c	=	Junge constant = 1.7×10^{-04} (atm-cm)
D_a	=	Diffusivity of COPC in air (cm^2/s)
D_w	=	Diffusivity of COPC in water (cm^2/s)
$f_{oc,bs}$	=	Fraction of organic carbon in bottom sediment (unitless)
$f_{oc,s}$	=	Fraction of organic carbon in soil (unitless)
$f_{oc,sw}$	=	Fraction of organic carbon in suspended sediment (unitless)
f_{water}	=	Fraction of COPC in water (unitless)

F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
Fw	=	Fraction of wet deposition that adheres to plant surfaces (unitless)
H	=	Henry's law constant
Inhalation CSF	=	Inhalation cancer slope factor $(mg/kg\text{-}day)^{-1}$
Inhalation URF	=	Inhalation unit risk factor $(\mu g/m^3)^{-1}$
Kd_s	=	Soil-water partition coefficient (mL water/g soil OR cm^3 water/g soil)
Kd_{sw}	=	Suspended sediment-surface water partition coefficient (L water/kg suspended sediment OR cm^3 water/g suspended sediment)
Kd_{bs}	=	Bed sediment-sediment pore water partition coefficient (L water/kg bottom sediment OR cm^3 water/g bottom sediment)
K_{ow}	=	Octanol/water partitioning coefficient (mg COPC/L octanol)/(mg COPC/L octanol)—unitless
K_{oc}	=	Soil organic carbon-water partition coefficient (mL water/g soil)
ksg	=	COPC soil loss constant due to biotic and abiotic degradation (yr^{-1})
MW	=	Molecular weight of COPC (g/mole)
p°_L	=	Liquidphase vapor pressure of COPC (atm)
p°_S	=	Solid-phase vapor pressure of COPC (atm)
Oral CSF	=	Oral cancer slope factor $(mg/kg\text{-}day)^{-1}$
R	=	Universal gas constant $(atm\text{-}m^3/mol\text{-}K)$
RCF	=	Root concentration factor (µg COPC/g DW plant)/(µg COPC/mL soil water)
RfC	=	Reference concentration (mg/m^3)
RfD	=	Reference dose (mg/kg/day)
Rp	=	Interception factor of edible portion of plant (unitless)
S	=	Solubility of COPC in water (mg COPC/L water)
ΔS_f	=	Entropy of fusion [$\Delta S_f/R$ = 6.79 (unitless)]
S_T	=	Whitby's average surface area of particulates (aerosols) = 3.5×10^{-06} cm^2/cm^3 air for background plus local sources = 1.1×10^{-05} cm^2/cm^3 air for urban sources
$t_{1/2}$	=	Half-time of COPC in soil (days)
T_a	=	Ambient air temperature (K)
T_m	=	Melting point temperature (K)
TEF	=	Toxicity equivalency factor (unitless)
Vp	=	Vapor pressure of COPC (atm)

APPENDIX A-2

The following sections provide the methodology and rationale followed for the selection or development of compound-specific parameter values recommended by U.S. EPA OSW. Compound-specific values are provided for (1) physical and chemical properties, (2) fate-and-transport parameters, and (3) health benchmarks. A summary table of all compound-specific parameter values is provided at the end of this appendix, followed by individual parameter-value tables for each compound. The individual parameter-value tables cite sources for each parameter value.

A2.1 PRIMARY GUIDANCE DOCUMENTS

Throughout Appendix A-2, the following guidance documents are referenced as the primary sources for the development and comparision of compound-specific parameter values, and used to the fullest extent possible to provide consistency. Therefore, in this appendix, the term **primary guidance documents** refers to the following documents:

- U.S. EPA. 1994f. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes: Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities.* Office of Emergency and Remedial Response (OERR). Office of Solid Waste. December 14.

- U.S. EPA. 1995b. *Review Draft Development of Human Health Based and Ecologically Based Exit Criteria for the Hazardous Waste Identification Project*. Volumes I and II. Office of Solid Waste. March 3.

- North Carolina Department of Environment, Health, and Natural Resources (NC DEHNR). 1997. *North Carolina Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units*. January.

To ensure consistency, sources referenced in the primary guidance documents were also evaluated. Information for certain compounds like PCDDs, PCDFs, and mercury were obtained from the following documents:

- U.S. EPA. 1994a. *Estimating Exposure to Dioxin-Like Compounds*. External Review Draft Report. Volumes I-III. Office of Research and Development. Washington, DC. EPA/600/6-88/005Ca,b,c.

- U.S. EPA. 1997g. *Mercury Study Report to Congress. Volume III: Fate and Transport of Mercury in the Environment.* Office of Air Quality Planning and Standards and Office of Research and Development. EPA-452/R-97-005. December.

U.S. EPA (1994a) provides various parameter values for (but are not limited to) PCDDs, PCDFs, and PCBs. U.S. EPA (1997g) provides various parameter values for mercuric compounds including elemental mercury, mercuric chloride, and methyl mercury.

A2.2 GENERAL ANALYSIS AND METHODOLOGY

This section describes the general analysis and methodology followed for the development of compound-specific parameter values presented. Compound-specific parameter values in the primary guidance documents and other sources generally were evaluated as follows:

1. Compound-specific values for each parameter were compared among the primary guidance documents and the following observations were noted:

    a. Parameter values provided in U.S. EPA (1994f) are limited to 24 compounds. For these compounds, sources were referenced specifically to each parameter, in addition to the methodology used to obtain the respective values.

    b. U.S. EPA (1995b) provides various parameter values for a comprehensive list of compounds. The methodology used for determining values was covered in detail. However, parameter values for each compound were not referenced to a specific source. Although a comprehensive list of sources was provided, it is difficult to determine which parameter value for a compound was obtained from which source.

    c. NC DEHNR (1997) provides various parameter values for a comprehensive list of compounds, including congeners of polychlorinated dibenzo(p)dioxins (PCDDs) and polychlorinated dibenzofurans (PCDFs). However, the sections citing the methodology and sources of values in the NC DEHNR (1997) were reproduced directly from U.S. EPA (1994f). Therefore, in NC DEHNR (1997), the compound-specific parameter values that were provided did not correlate with the sections citing the methodology and sources of values. In addition, only a partial list of sources was provided for the values. Therefore, it was not possible to determine the actual source of values with certainty.

2. Sources of values referenced in the primary guidance documents were further researched and evaluated. Observations affecting usability are included in parameter-specific discussions for each compound, as appropriate.

3. Values provided in the primary guidance documents were used only when the sources and applicability of such values could be verified. Additional sources of parameter values were evaluated, used, and referenced when technically justified.

4. Recommended parameter values obtained using correlations or equations were calculated using the recommended values for these variables provided in this SLERAP.

In general, for the selection of parameter values, the following three steps were followed:

1. Whenever measured parameter values were available in published literature studies, they were preferred for use over other types of data. When multiple measured values were available, the geometric mean of the parameter values is recommended for use.

2. In the absence of measured values in published literature that could not be directly evaluated, parameter values compiled or adopted for use by the primary guidance

documents, U.S. EPA (1994a), and U.S. EPA (1997g) are recommended.

3. If unable to obtain acceptable values from published literature or the primary guidance documents, parameter values were estimated or calculated using correlation equations based on sound scientific judgment.

The following sections, A2.3 through A2.5, provide compound-specific parameter values, which are categorized and discussed as follows: (1) organic compounds, including polychlorinated biphenyls (PCB), and excluding methyl mercury, PCDDs and PCDFs, (2) PCDDs and PCDFs, (3) all metals except mercury, and (4) the mercuric compounds—mercury (elemental; metal), mercuric chloride (divalent inorganic mercury), and methyl mercury (organic mercury).

For each of the parameters, the sources of values referenced in this SLERAP are followed by a discussion and justification of their selection. There is also a brief discussion of the methodology followed by each of the primary guidance documents. This provides a complete evaluation and comparison of the compound-specific parameter values provided in the primary guidance documents that are currently used to conduct risk assessments.

A2.3 PHYSICAL AND CHEMICAL PROPERTIES

A2.3.1 Molecular Weight (*MW*)

Molecular weight (*MW*) of a compound is defined as the sum of atomic weights of all atoms in the compound's molecule.

Organics and Metals For most organics (except PCDDs and PCDFs) and metals, this SLERAP provides *MW* values that were obtained from the following:

- Budavari, S., M.J. O'Neil, A. Smith, and P.E. Heckelman. 1989. *The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals.* 11th Edition. Merck and Company, Inc. Rahway, New Jersey.

MW values not provided in Budavari, O'Neil, Smith, and Heckelman (1989) were obtained from the following document:

- Montgomery, J.H., and L.M. Welkom. 1991. *Groundwater Chemicals Desk Reference.* Lewis Publishers. Chelsea, Michigan.

Because Budavari, O'neil, Smith, and Heckelman (1989) provides *MW* values for most of the compounds evaluated, it was used as the primary source to ensure consistency. *MW* values are based on the compound's formula; and, the values in Budavari, O'Neil, Smith, and Heckelman (1989) are the same as the values cited in several literature sources. *MW* values for most of the compounds in the primary guidance documents were also obtained from Budavari, O'Neil, Smith, and Heckelman (1989).

PCDDs and PCDFs *MW* values for PCDDs and PCDFs were obtained from U.S. EPA (1994a).

Mercuric Compounds *MW* values for mercury and mercuric chloride were obtained from Budavari and others (1989). *MW* value for methyl mercury was obtained from U.S. EPA (1997g).

A2.3.2 Melting Point Temperature (T_m)

Melting point temperature (T_m) is the temperature of the compound (in degree Kelvin [K]) at which the solid state of the compound undergoes a phase change to a liquid phase. At ambient temperatures and at an atmpospheric pressure of 1 atmosphere, compounds are either in a solid or liquid state. The compound liquid or solid state is provided in the summary tables of compound-specific parameter values.

Organics and Metals For most organics (except PCDDs and PCDFs) and metals, this SLERAP provides values for T_m that were obtained from Budavari, O'Neil, Smith, and Heckelman (1989). T_m values not provided in Budavari, O'Neil, Smith, and Heckelman (1989) were obtained from Montgomery and Welkolm (1991).

Because Budavari, O'Neil, Smith, and Heckelman (1989) provides T_m values for most of the compounds evaluated, it was used as the primary source to ensure consistency. T_m values in Budavari, O'Neil, Smith, and Heckelman (1989) were generally within 2 to 3 degrees of the values provided in literature sources reviewed. T_m values for most compounds in the primary guidance documents were also obtained from Budavari, O'Neil, Smith, and Heckelman (1989).

PCDDs and PCDFs *Tm* values for PCDDs and PCDFs were obtained from U.S. EPA (1994a). U.S. EPA (1994a) provides T_m values for PCDDs and PCDFs, that were obtained from various literature sources.

A2.3.3 Vapor Pressure (*Vp*) and Aqueous Solubility (*S*)

The vapor pressure (*Vp*) of a substance is defined as the pressure in atmospheres exerted by the vapor (gas) of a compound when it is under equilibrium conditions. It provides a semi-quantitative rate at which it will volatilize from soil and/or water. The aqueous solubility (*S*) of a compound is defined as the saturated concentration of the compound in water (mg COPC/L water) at a given temperature and pressure, usually at soil/water temperatures and atmospheric pressure (Montgomery and Welkom 1991).

Organics For most organics (except PCDDs and PCDFs), values for *Vp* and *S* were obtained from the following:

- U.S. EPA 1994c. *Draft Report Chemical Properties for Soil Screening Levels*. Prepared for the Office of Emergency and Remedial Response. Washington, DC. July 26.

U.S. EPA (1994c) provides measured, calculated, and estimated values for *Vp* and *S* that were obtained from various literature sources. *Vp* values in U.S. EPA (1994c) were generally either measured (at 20°C to 25°C) or calculated values obtained from various literature sources. U.S. EPA (1994c), however, provides values for *Vp* corrected to 25°C. U.S. EPA (1995b) states that, because the distribution of many of the parameters is skewed, the geometric mean or the median values were preferable to the arithmetic mean values. Therefore, when available geometric mean values were preferred over the arithmetic mean values. The geometric mean of the temperature corrected *Vp* values, determined from measured and calculated values, is recommended for use in this SLERAP.

In U.S. EPA (1994c), *S* values were either measured (at 20°C to 30°C) or calculated values obtained from various literature sources. The geometric mean *S* value, calculated from measured and calculated values, is recommended for use in this SLERAP. Although *S* values were measured at temperatures ranging

from 20°C to 30°C, U.S. EPA (1994c) states that *S* values were not corrected to 25°C, because the variability in solubilities measured at 20°C to 25°C was within the overall range of measured values.

U.S. EPA (1994c) is the preferred source, because (1) sources and the conditions at which each value was obtained are provided, and (2) values were provided to 2 significant figures. Also, U.S. EPA (1994c) provides multiple *Vp* and *S* values for each compound from several different literature sources; providing a recent, more comprehensive compilation of reported literature values. *Vp* and *S* values from U.S. EPA (1994c) were generally consistent with those provided in U.S. EPA (1994f), U.S. EPA (1995b), and NC DEHNR (1997).

When *Vp* and *S* values were not available in U.S. EPA (1994c), they were obtained from one of three sources, in the following order of preference:

1. U.S. EPA (1994f)

2. U.S. EPA (1995b); values from which were obtained from one of three sources:

    a. Mackay, D., W.Y. Shiu, and K.C. Ma. 1992. *Illustrated Handbook of Physical-Chemical Properties and Environmental fate for Organic Chemicals. Volume I - Monoaromatic Hydrocarbons, Chlorobenzenes, and PCBs. Volume II-Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins and Dibenzofurans. Volume III - Volatile Organic Chemicals.* Lewis Publishers. Boca Raton, Florida.

    b. Howard, P.H. 1989-1993. *Handbook of Environmental Fate and Exposure Data For Organic Chemicals*. *Volumes I: Large Production and Priority Pollutants (1989). Volume II: Solvents (1990). Volume III: Pesticides (1991). Volume IV: Solvents2 (1993).* Lewis Publishers. Chelsea, Michigan.

    c. Other referenced literature sources, when values were not available in Mackay, Shiu, and Ma (1992) or Howard (1989-1993).

3. U.S. EPA. 1994b. *Superfund Chemical Data Matrix (SCDM).* Office of Emergency and Remedial Response. Washington, DC. June.

Vp and *S* values in U.S. EPA (1994f) were geometric mean values obtained from various literature sources. References specific to sources of values for each compound were provided in U.S. EPA (1994f) and were, therefore, preferred over U.S. EPA (1995b) values.

Most *Vp* and *S* values in U.S. EPA (1995b) were obtained from Mackay, Shiu, and Ma (1992) or Howard (1989-1993). Mackay, Shiu, and Ma (1992) and Howard (1989-1993) obtain the "best" values after evaluation of various literature sources.

Vp values in U.S. EPA (1994b) were obtained from various literature sources. *S* values in U.S. EPA (1994b) were the geometric mean of values obtained from various literature sources.

PCDDs and PCDFs *Vp* and *S* values for PCDDs and PCDFs were obtained from U.S. EPA (1994a). *Vp* and *S* values were either (1) measured, or (2) estimated by using the homologue (compound class with the same amount of chlorination) average method.

NOTE: The phase—solid or liquid—of *Vp* values for all organics, including PCDDs and PCDFs, was indicated. This is based on whether the compound is in the solid or liquid phase at ambient soil temperatures.

Metals As cited in the primary guidance documents and in the literature, metals—except mercury—are considered (1) nonvolatile at ambient temperatures, and (2) insoluble in water, except as certain weak acids. Therefore, *Vp* and *S* values were not available for all metals (except mercury) in any of the literature sources reviewed.

Mercuric Compounds Mercury is a relatively volatile compound. *Vp* and *S* values for elemental mercury were obtained from Budavari, O'Neil, Smith, and Heckelman (1989); and are comparable to the values in the primary guidance documents. *Vp* and *S* values for mercuric chloride were obtained from U.S. EPA (1997g) and Budavari, O'Neil, Smith, and Heckelman (1989), respectively. *Vp* and *S* values for methyl mercury were not found in the literature.

A2.3.4 Henry's Law Constant (*H*)

Henry's Law constant (*H*) is also referred to as the air-water partition coefficient, and is defined as the ratio of the partial pressure of a compound in air to the concentation of the compound in water at a given temperature under equilibrium conditions. Henry's Law constant values generally can be (1) calculated from the theoretical equation defining the constant, (2) measured, or (3) estimated from the compound structure. Experimental and estimated *H* values from literature reports, however, are (1) very temperature-dependent and difficult to measure, (2) generally obtained from various literature sources that use different experimental and estimation methods, and (3) available for only a limited number of compounds.

Organics For organics (excluding PCDDs and PCDFs), *H* values were calculated from the following theoretical equation (Lyman, Reehl, and Rosenblast 1982) for consistency, using recommended *MW*, *S*, and *Vp* values provided in this SLERAP:

$$H = \frac{Vp \cdot MW}{S} \qquad \text{Equation A2-1}$$

H	=	Henry's Law constant (atm-m^3/mole)
Vp	=	Vapor pressure of COPC (atm)
S	=	Solubility of COPC in water (mg COPC/L water)

The primary guidance documents also used theoretical Equation A-3-1 to calculate *H* values.

PCDDs and PCDFs *H* values for PCDDs and PCDFs are calculated values obtained from U.S. EPA (1994a).

Metals For all metals (except mercury), *H* is zero, because *Vp*—because of the nonvolatile nature of the metals—and *S* are assumed to be zero.

Mercuric Compounds *H* values for elemental mercury, mercuric chloride, and methyl mercury were obtained from U.S. EPA (1997g).

A2.3.5 Diffusivity of COPCs in Air (D_a) and Water (D_w)

Diffusivity or diffusion coefficients in air (D_a) and water (D_w) are used to calculate the liquid or gas phase transfer of a COPC into a waterbody.

Organics For organics (except PCDDs and PCDFs), diffusivity values were obtained directly from the CHEMDAT8 model chemical properties database (Worksheet DATATWO.WK1):

- U.S. EPA. 1994d. *CHEM8—Compound Properties Estimation and Data*. Version 1.00. CHEMDAT8 Air Emissions Program. Prepared for Chemicals and Petroleum Branch, OAQPS. Research Triangle Park. North Carolina. November 18.

The U.S. EPA (1994d) database uses empirical correlations with compound density and molecular weight to calculate diffusivity values. For compounds not in the U.S. EPA (1994d) database, diffusivity values were obtained by using the WATER8 model correlation equations for air and water diffusivities:

- U.S. EPA. 1995d. *WATER8—Air Emissions Models Wastewater Treatment*. Version 4.0. OAQPS. Research Triangle Park. North Carolina. May 1.

U.S. EPA(1995d) database values were predicted by using chemical-structural relationships. Diffusivity values for all compounds in the U.S. EPA (1994d) and (1995d) databases were either predicted or estimated. The primary guidance documents also recommended U.S. EPA (1994d) and (1995d) database model values. More recent documents, including the following, also recommended these values:

- U.S. EPA. 1996. *Soil Screening Guidance: Technical Background Document and User's Guide*. Office of Solid Waste and Emergency Response. Washington, DC. EPA/540/R-95/128. May.

For diffusivity values that were not available in these databases, D_w and D_a values were calculated using the following equations cited and recommended for use in U.S. EPA (1997g):

$$D_{a,i} = \frac{1.9}{(MW_i)^{2/3}} \qquad \text{Equation A2-2a}$$

$$D_{w,i} = \frac{22\times10^{-5}}{(MW_i)^{2/3}} \qquad \text{Equation A2-2b}$$

U.S. EPA (1995b) recommended the use of standard default diffusivity values. U.S. EPA (1995b) stated that the diffusivity parameters vary slightly, and default values appear to be within the range of typical values. Values for diffusivity in air range from about 0.01 to 0.1 square centimeters per second (cm^2/s); therefore, U.S. EPA (1995b) recommended a default value of 0.08 cm^2/s. Values for diffusivity in water range from 1×10^{-06} to 1×10^{-05} cm^2/s; therefore, U.S. EPA (1995b) recommended a default value of 8×10^{-06} cm^2/s. Diffusivity values calculated using Equations A-2-2a and A-2-2b were within the range specified by U.S. EPA (1995b), and therefore, were adopted for use in this SLERAP.

PCDDs and PCDFs Diffusivity values in air and water for (1) 2,3,7,8-TCDD were obtained from U.S. EPA (1994e), and (2) 2,3,7,8-TCDF were obtained from U.S. EPA (1995d). For all other congeners of PCDDs and PCDFs, (1) a default *Dw* value of 8×10^{-06} cm^2/s was used, and (2) *Da* values were calculated using the following equation recommended by U.S. EPA (1994a):

$$\frac{D_x}{D_y} = \left(\frac{MW_y}{MW_x}\right)^{0.5} \qquad \text{Equation A2-2c}$$

where

$D_{x,y}$ = Diffusivities in air of compounds *x* and *y* (cm^2/s)
$MW_{x,y}$ = Molecular weights of compounds *x* and *y* (g/mol)

Da values for PCDD congeners were calculated by using the *Da* value and *MW* for 2,3,7,8-TCDD. *Da* values for PCDF congeners were calculated using the *Da* value and *MW* for 2,3,7,8-TCDF. This approach is consistent with the methodology specified in U.S. EPA (1994a).

Metals and Mercuric compounds For metals (except chromium and mercury), diffusivity values were not available in the literature. Diffusivity values for chromium and mercury were obtained from the U.S. EPA (1994d) database. Diffusivity values for mercuric chloride and methyl mercury were calculated using Equations A-2-2a and A-2-2b.

A2.3.6 Octanol/Water Partitioning Coefficient (K_{ow})

The *n*-octanol/water partitioning coefficient (K_{ow}) is defined as the ratio of the solute concentration in the water-saturated *n*-octanol phase to the solute concentration in the *n*-octanol-saturated water phase (Montgomery and Welkom 1991).

Organics For organics (except PCDDs and PCDFs), K_{ow} values were obtained from U.S. EPA (1994c). U.S. EPA (1994c) provides measured, calculated, and estimated K_{ow} values obtained from various literature sources. The geometric mean K_{ow} value, calculated from all measured and calculated values for each compound, is recommended in this SLERAP.

K_{ow} values that were not available in U.S. EPA (1994c) were obtained from one of three sources, in the following order of preference:

1. U.S. EPA (1994f)

2. Karickhoff, S.W. and J.M. Long. 1995. "Internal Report on Summary of Measured, Calculated, and Recommended Log K_{ow} Values." Environmental Research Laboratory. Athens. April 10.

3. U.S. EPA (1995b), values from which were obtained from one of three sources:

   a. Mackay, D., W.Y. Shiu, and K.C. Ma. 1992. *Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Volume I - Monoaromatic Hydrocarbons, Chlorobenzenes, and PCBs. Volume II - Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins and Dibenzofurans. Volume III - Volatile Organic Chemicals.* Lewis Publishers. Boca Raton, Florida.

   b. Howard, P.H. 1989-1993. *Handbook of Environmental Fate and Exposure Data For Organic Chemicals*. *Volumes I: Large Production and Priority Pollutants (1989). Volume II: Solvents (1990). Volume III: Pesticides (1991). Volume IV: Solvents2 (1993).* Lewis Publishers. Chelsea, Michigan.

   c. Other literature sources, when values were not available in Mackay, Shiu, and Ma (1992) and Howard (1989-1993).

U.S. EPA (1994c) is the preferred source of values because (1) sources were provided, (2) several literature values were provided, some of which are also cited by the primary guidance documents and Karickhoff and Long (1995), and (3) the values were provided to 2 significant figures.

U.S. EPA (1994f) is the second-choice source of K_{ow} values recommended; and provides geometric mean values obtained from various literature sources. Karickhoff and Long (1995) recommended arithmetic mean values obtained from various literature sources and was, therefore, preferred as the third-choice source of K_{ow} values when values were not available from the first two sources.

In order to reference specific sources of K_{ow} values for each compound, values from U.S. EPA (1995b) and NC DEHNR (1997) were used only when values were not available in the literature sources reviewed.

PCDDs and PCDFs K_{ow} values for the PCDDs and PCDFs were obtained from either U.S. EPA (1994a) or U.S. EPA (1992d). U.S. EPA (1994a) and U.S. EPA (1992d) provide K_{ow} values for PCDDs and PCDFs that were either measured values obtained from the literature or calculated by averaging the literature values within the homologue group. According to U.S. EPA (1994a), K_{ow} values for hexachlorodibenzofurans were not available in the literature. Therefore, as recommended in U.S. EPA (1994a), due to lack of data, homologue group average values for hexachlorodibenzodioxins were applied to hexachlorodibenzofurans.

Metals No K_{ow} values were available for metals, either in the literature or in the primary guidance documents. K_{ow} values for the metals were assumed to be zero, because the affinity of the metals to the octanol is almost zero.

Mercuric compounds No K_{ow} values were available in the literature for mercury and methyl mercury. For mercuric chloride, the K_{ow} value was obtained from U.S. EPA (1997g).

A2.3.7 Soil Organic Carbon-Water Partition Coefficient (K_{oc})

The soil organic carbon-water partition coefficient (K_{oc}) or the organic carbon normalized soil sorption coefficient is defined as the ratio of adsorbed compound per unit weight of organic carbon to the aqueous solute concentration (Montgomery and Welkom 1991).

Organics Because of the soil mechanisms that are inherently involved, K_{oc} values for the ionizing organics and nonionizing organics are discussed separately.

A2.3.7.1 Ionizing Organic Compounds

Ionizing organic compounds include amines, carboxylic acids, and phenols. These compounds contain the functional groups that ionize under specific pH conditions, and include the following:

- Organic acids (2,4,6-trichlorophenol; pentachlorophenol; 2,3,4,5-tetrachlorophenol; 2,3,4,6-tetrachlorophenol; 2,4,5-trichlorophenol; 2,4-dichlorophenol; 2-chlorophenol; phenol; 2,4-dimethylphenol; 2-methylphenol; 2,4-dinitrophenol; and benzoic acid)

- Organic bases—n-nitroso-di-n-propylamine; n-nitrosodiphenylamine, and 4-chloroaniline)

K_{oc} values for ionizing organic compounds were obtained from U.S. EPA (1994c). U.S. EPA (1994c) provides K_{oc} values for the ionizing organic compounds that have been estimated on the basis of the degree of ionization and the relative proportions of neutral and ionized species. The primary guidance documents cite one value for the ionizing organics, independent of the pH. The primary guidance documents calculate K_{oc} values for the ionizing organics by using correlation equations containing K_{ow} that are applicable to nonionizing organics. However, K_{oc} values for ionizing compounds can vary vastly, depending on the pH conditions in the environment. Therefore, for the aforementioned ionizing organic compounds, this SLERAP prefers and provides estimated K_{oc} values that are based on pH.

K_{oc} values were estimated on the basis of the assumption that the sorption of ionizing organic compounds is similar to hydrophobic organic sorption, because the soil organic carbon is the dominant sorbent. According to U.S. EPA (1994c), for low pH conditions, these estimated values may overpredict sorption coefficients, because they ignore sorption to components other than organic carbon.

A2.3.7.2 Nonionizing Organic Compounds

Nonionizing organic compounds are all other organic compounds not listed earlier as ionizing. They include volatile organics, chlorinated pesticides, polynuclear aromatic hydrocarbons (PAHs), and phthalates. This SLERAP uses geometric mean of measured K_{oc} values provided in the following document:

- U.S. EPA. 1996b. *Soil Screening Guidance: Technical Background Document and User's Guide*. Office of Solid Waste and Emergency Response. Washington, DC. EPA/540/R-95/128. May.

U.S. EPA (1996b) calculated the geometric mean value from various measured values. For compounds for which K_{oc} values are not provided by U.S. EPA (1996b), K_{oc} values were calculated using K_{ow} correlation equations provided in the same document.

NC DEHNR (1997) and U.S. EPA (1994f) use the following correlation equation to calculate K_{oc} from K_{ow} for all organics:

$$\log K_{oc} = 0.88 (\log K_{ow}) + 0.114 \qquad (r^2 = 0.96) \qquad \text{Equation A-2-3}$$

- Research Triangle Institute (RTI). 1992. *Preliminary Soil Action Level for Superfund Sites, Draft Interim Report.* Prepared for U.S. EPA Hazardous Site Control Division, Remedial Operations Guidance Branch. Arlington, Virginia. December.

However, according to U.S. EPA (1994c), the correlation between K_{oc} and K_{ow} can be improved considerably by performing separate linear regressions on two chemical groups. U.S. EPA (1994c) derives the following correlation equations from measured K_{oc} values cited in U.S. EPA (1994c) and U.S. EPA (1996b):

For phthalates and PAHs

$$\log K_{oc} = 0.97 (\log K_{ow}) - 0.094 \qquad (r^2 = 0.99) \qquad \text{Equation A-2-4}$$

For all organics except phthalates, PAHs, PCDDs, and PCDFs

$$\log K_{oc} = 0.78 (\log K_{ow}) + 0.151 \qquad (r^2 = 0.98) \qquad \text{Equation A-2-5}$$

Because of the improved regressions (r^2), U.S. EPA (1994c) recommended that correlation Equations A-2-4 and A-2-5 be used instead of correlation Equation A-2-3. U.S. EPA (1995b) also recommended that correlation Equations A-2-4 and A-2-5 be used.

Although U.S. EPA (1995b) recommended the use of correlation Equations A-2-4 and A-2-5, the following correlation equation was used by that document to calculate K_{oc} values for all organics except PCDDs and PCDFs:

$$\log K_{oc} = 0.983 (\log K_{ow}) + 0.0002 \qquad \text{Equation A-2-6}$$

- DiToro, D.M., C.S. Zarba, D.J. Hansen, W.J. Berry, R.C. Swartz, C.E. Cowan, S.P. Pavlou, H.E. Allen, N.A. Thomas, and P.R. Paquin. 1991. "Technical Basis for

Establishing Sediment Quality Criteria for Nonionic Compounds Using Equilibrium Partitioning." *Environmental Toxicology and Chemistry*. 10:1541-1583

For the purposes of this SLERAP, values obtained by using correlation Equations A-2-3 through A-2-6, were compared. In general, more of the K_{oc} values obtained by using correlation Equations A-2-4 and A-2-5 were within the range of measured values in the literature than those obtained by using correlation Equations A-2-3 and A-2-6. Therefore, when measured K_{oc} values were not available, values were estimated, for all nonionizing organic compounds except PCDDs and PCDFs, by using the appropriate correlation Equation A-2-4 or A-*2-5*.

PCDDs and PCDFs For PCDDs and PCDFs, the following correlation equation (Karickhoff, Brown, and Scott 1979) was used to calculate K_{oc} values, as cited by U.S. EPA (1994a).

$$\log K_{oc} = \log K_{ow} - 0.21 \qquad (n = 10,\ r^2 = 1.0) \qquad \text{Equation A-2-7}$$

- Karickhoff, S.W., D.S. Brown, and T.A. Scott. 1979. "Sorption of Hydrophobic Pollutants on Natural Sediments." Water Resources. 13:241-248.

Metals For metals, no K_{oc} values were found in the literature. K_{oc} values for metals were not provided in the primary guidance documents, because of the stated assumption that organic carbon in soils does not play a major role in partitioning in soil and sediments. For metals, soil/sediment-water partitioning coefficients (*Kd*) were obtained directly from experimental measurements (see *Kd* discussion).

Note: For compounds in which a K_{ow} correlation equation was used to calculate a K_{oc} value, K_{ow} values recommended for each compound in this SLERAP were used.

A2.3.8 Partitioning Coefficients for Soil-Water (Kd_s), Suspended Sediment-Surface Water (Kd_{sw}), and Bottom Sediment-Sediment Pore Water (Kd_{bs})

Partition coefficients (*Kd*) describe the partitioning of a compound between sorbing material, such as soil, soil pore-water, surface water, suspended solids, and bed sediments. For organic compounds, *Kd* has been estimated to be a function of the organic-carbon partition coefficient and the fraction of organic carbon in the partitioning media. For metals, *Kd* is assumed to be independent of the organic carbon in the partitioning media and, therefore, partitioning is similar in all sorbing media.

The soil-water partition coefficient (Kd_s) describes the partitioning of a compound between soil pore-water and soil particles, and strongly influences the release and movement of a compound into the subsurface soils and underlying aquifer. The suspended sediment-surface water partition coefficient (Kd_{sw}) coefficient describes the partitioning of a compound between surface water and suspended solids or sediments. The bed sediment-sediment pore-water partition coefficient (Kd_{bs}) coefficient describes the partitioning of a compound between the bed sediments and bed sediment pore-water.

Organics For organics (including PCDDs and PCDFs), soil organic carbon is assumed to be the dominant sorbing component in soils and sediments. Therefore, *Kd* values were calculated using the following fraction organic carbon (f_{OC}) correlation equations:

$$Kd_s = f_{oc,s} \cdot K_{oc} \qquad \text{Equation A-2-8a}$$

$$Kd_{sw} = f_{oc,sw} \cdot K_{oc} \qquad \text{Equation A-2-8b}$$

$$Kd_{bs} = f_{oc,bs} \cdot K_{oc} \qquad \text{Equation A-2-8c}$$

- U.S. EPA. 1993d. Review Draft Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions. Office of Health and Environmental Assessment. Office of Research and Development. EPA-600-AP-93-003. November 10.

U.S. EPA (1993d), from literature searches, states that f_{OC} could range as follows:

- 0.002 to 0.024 in soils—for which a mid-range value of $f_{oc,s}$ = 0.01 generally can be used.
- 0.05 to 0.1 in suspended sediments—for which a mid-range value of $f_{oc,sw}$ = 0.075 generally can be used.
- 0.03 to 0.05 in bottom sediments—for which a mid-range value of $f_{oc,bs}$ = 0.04 generally can be used.

Consistent with the primary guidance documents, this SLERAP uses mid-range f_{oc} values recommended by U.S. EPA (1993d). *Kd* values were calculated using K_{oc} values recommended for each compound in this SLERAP.

Metals For metals (except mercury), *Kd* is governed by factors other than organic carbon, such as pH, redox, iron content, cation exchange capacity, and ion-chemistry. Therefore, *Kd* values for metals cannot be calculated using the same correlation equations specified for organic compounds. Instead, *Kd* values for the metals must be obtained directly from literature sources. *Kd* values for all metals, except lead, were obtained from U.S. EPA (1996b). U.S. EPA (1996b) provides values for *Kd* that are based on pH, and are estimated by using the MINTEQ2 model, which is a geochemical speciation model. The MINTEQ2 model analyses were conducted under a variety of geochemical conditions and metal concentrations. The MINTEQ2 pH-dependent *Kd* values were estimated by holding constant the iron oxide at a medium value and the f_{oc} at 0.002. For arsenic, hexavalent chromium, selenium, and thallium, empirical pH-dependent *Kd* values were used.

U.S. EPA (1995b) also recommended *Kd* values estimated using the MINTEQ2 model. U.S. EPA (1994f) and NC DEHNR (1997) provided *Kd* values obtained from several literature sources, depending on the compound; however, the *Kd* values are identical in all of the primary guidance documents.

The MINTEQ2 model values in U.S. EPA (1996b) were comparable to the values in the primary guidance documents. In addition, because organic carbon does not play a major role in partitioning for the metals, U.S. EPA (1994f) assumed that the partitioning is the same, regardless of the soil, suspended

sediment, or bottom sediment phase. Therefore, in this SLERAP, values for partitioning coefficients Kd_s, Kd_{sw}, and Kd_{bs} for the metals are assumed to be the same.

Kd value for lead was obtained from the following*:*

- Baes, C.F., R.D. Sharp, A.L. Sjoreen, and R.W. Shor. 1984. "Review and Analysis of Parameters and Assessing Transport of Environmentally Released Radionuclides Through Agriculture." Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Mercuric Compounds Kd_s, Kd_{sw}, and Kd_{bs} values for mercury, mercuric chloride, and methyl mercury were obtained from U.S. EPA (1996b). Kd values for mercuric chloride and methyl mercury were obtained from U.S. EPA (1997g).

A2.3.9 Soil Loss Constant Due to Degradation *(ksg)*

Soil loss constant due to degradation *(ksg)* reflects loss of a compound from the soil by processes other than leaching. Degradation rates in the soil media include biotic and abiotic mechanisms of transformation. Abiotic degradation includes photolysis, hydrolysis, and redox reactions. Hydrolysis and redox reactions can be significant abiotic mechanisms in soil (U.S. EPA 1990).

The following document states that degradation rates can be assumed to follow first order kinetics in a homogenous media:

- Lyman , W.J., W.F. Reehl, and D.H. Rosenblatt. 1982. *Handbook of Chemical Property Estimation Methods: Environmental Behavior of Organic Compounds.* McGraw-Hill Book Company. New York, New York.

Therefore, the half-life $(t_{½})$ of compounds can be related to the degradation rate constant (*ksg*) as follows:

$$ksg = \frac{0.693}{t_{½}} \qquad \text{Equation A-2-9}$$

Ideally, *ksg* is the sum of all biotic and abiotic rate constants in the soil. Therefore, if the $t_{½}$ for all of the mechanisms of transformation are known, the degradation rate can be calculated using Equation A-2-9. However, literature sources generally do not provide sufficient data for all such mechanisms, especially for soil.

Organics For organics (except PCDDs and PCDFs), *ksg* values were calculated using half-life soil values obtained from the following document:

- Howard, P.H., Boethling, R.S., Jarvis, W.F., Meylan, W.M., and Michalenko, E.M. 1991. *Handbook of Environmental Degradation Rates.* Lewis Publishers. Chelsea, Michigan.

Half-life values provided in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) indicate the disappearance of a substance in ground water or soil; with the principal degradation mechanisms being

biodegradation and hydrolysis. Values reported were highly variable because of the different methods used for measurements, in addition to the various controlling factors that could affect them. Therefore, Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) provided a range of half-life values found in the literature, usually for the fastest reaction mechanism,. *Ksg* values recommended in this SLERAP were calculated with the high-end half-life values.

U.S. EPA (1994b) also cited values obtained from Howard, Boethling, Jarvis, Meylan, and Michalenko (1991). NC DEHNR (1997) cited values that are comparable to *ksg* values calculated by using half-life values obtained from Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).

PCDDs and PCDFs For PCDDs and PCDFs, *ksg* values were calculated from half-life values in soil obtained from Mackay, Shiu, and Ma (1992). For 2,3,7,8-TCDD, *ksg* value was obtained from U.S. EPA (1994a); which discussed experimental studies that were conducted on PCDDs and PCDFs degradation mechanisms. U.S. EPA (1994a) summarized the degradation of PCDDs and PCDDs as follows:

- A few experimental studies have shown possible biological degradation of TCDDs. However, the studies conclude that microbial action is very slow for PCDDs under optimum conditions, with the degradation rates probably higher with decreasing chlorination. PCDFs were found to be extremely stable to biological degradation.

- Abiotic degradation, such as photolysis, appears to be the most significant natural degradation mechanism for PCDDs and PCDFs. Experimental studies have shown that PCDDs and PCDFs undergo photolysis in the presence of a suitable hydrogen donor. No information was available to show that other abiotic degradation mechanisms, such as oxidation and hydrolysis, are important under environmentally relevant conditions.

Metals For the metals, NC DEHNR (1997) cites *ksg* values of zero. Literature states that the metals are transformed, but not degraded, by such mechanisms; therefore, *ksg* values are not applicable to metals.

Mercuric Compounds For mercury, mercuric chloride, and methylmercury, U.S. EPA (1997g) recommended *ksg* values of zero.

A2.3.10 Fraction of Pollutant Air Concentration in the Vapor Phase (F_v)

Organics For organics, the fraction of pollutant air concentration in the vapor phase (F_v) was calculated using the following equation:

$$Fv = 1 - \frac{c\,S_T}{p^{\circ}_L + c\,S_T} \qquad \text{Equation A-2-10}$$

- Junge, C. E. 1977. *Fate of Pollutants in the Air and Water Environments*, Part I; Suffet, I. H., Ed.; Wiley; New York. Pages 7-26.

If the compound is a liquid at ambient temperatures (that is, when p°_L is known), Equation A-2-10 calculates F_v using the vapor pressure value recommended for that compound in this SLERAP. If the

compound is a solid at ambient temperatures (that is, when p°_S is known), the following equation (Bidleman 1988) was used to calculate p°_L from p°_S, for use in Equation A-2-10:

$$\ln\left(\frac{p^{\circ}_L}{p^{\circ}_S}\right) = \frac{\Delta S_f}{R}\,\frac{(T_m - T)}{T} \qquad \text{Equation A-2-11}$$

where

c	=	Junge constant = 1.7 x 10^{-04} (atm-cm)
p°_L	=	Liquid phase vapor pressure of compound (atm)
p°_s	=	Solid phase vapor pressure of compound (atm)
R	=	Universal ideal gas constant (atm-m^3/mole-K)
ΔS_f	=	Entropy of fusion [$\Delta S_f/R$ = 6.79 (unitless)]
S_T	=	Whitby's average surface area of particulates (aerosols)
T_a	=	Ambient air temperature (K)—assumed to be 25°C or 298 K

This equation was adopted from:

- Bidleman, T.F. 1988. "Atmospheric Processes." *Environmental Science and Technology.* Volume 22. Number 4. Pages 361-367.

According to Bidleman (1988), Equation A-2-10 assumes that the Junge constant (c) is constant for all compounds. However, c can depend on (1) the compound (sorbate) molecular weight, (2) the surface concentration for monolayer coverage, and (3) the difference between the heat of desorption from the particle surface and the heat of vaporization of the liquid-phase sorbate.

The primary guidance documents used Equations A-2-10 and A-2-11 to compute *Fv*. However, it is not clear what values of *S*, *T*, and *Vp* values were used to calculate values for F_v. For example, U.S. EPA (1994f) calculated F_v values at (T) of 11°C. Because of inconsistencies in the values in the primary guidance documents, *Fv* values in the primary guidance documents were not recommended for use in this SLERAP. F_v values were calculated using the recommended values of *Vp* and T_m provided in this SLERAP for each compound.

Metals Consistent with U.S. EPA (1994f), all metals (except mercury) are assumed to be present in the particulate phase and not in the vapor phase (*Vp* = 0), and assigned F_v values of zero.

Mercuric Compounds Mercury and mercuric chloride are relatively volatile and exist in the vapor phase (U.S. EPA 1997g). Therefore, the *Fv* value recommended in this SLERAP for mercury was calculated using Equations A-2-10 and A-2-11.

Based on discussions on mercury presented in Chapter 2 of this SLERAP, *Fv* values of 1.0 for mercury (same as calculated using Equations A-2-10 and A-2-11), and 0.85 for mercuric chloride were estimated. Consistent with information provided in U.S. EPA (1997g), methyl mercury is assumed not to exist in the air phase and, therefore, assigned an *Fv* of zero.

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ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 1 of 10)

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 2 of 10)

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 3 of 10)

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 4 of 10)

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 5 of 10)

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 6 of 10)

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 7 of 10)

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 8 of 10)

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 9 of 10)

ATTACHMENT

TABLES OF COMPOUND-SPECIFIC PARAMETER VALUES

(Page 10 of 10)

TABLE A-2-1

CHEMICAL-SPECIFIC INPUTS FOR ACENAPHTHENE (83-32-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	154.21
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	368.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.93E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.13E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.84E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.21E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.19E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	9.22E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.90E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value calculated using K_{oc} value provided in this table.	4.90E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.67E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.96E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.48E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-2

CHEMICAL-SPECIFIC INPUTS FOR ACETALDEHYDE (75-07-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	44.05
T_m (K)	Montgomery and Welkom (1991)	149.6
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.72E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.33E-05
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	6.02E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.53E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.53E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.15E-02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.81E-02
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0
Fv (unitless)	*Fv* value was assumed to be 1.0 due to a lack of data.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-3

CHEMICAL-SPECIFIC INPUTS FOR ACETONE (67-64-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	58.08
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	179.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.99E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	6.04E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.88E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.87E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.15E-05
K_{ow} (unitless)	Geometric mean value cited in Karickoff and Long (1995).	6.00E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.51E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.51E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.13E-02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-4

CHEMICAL-SPECIFIC INPUTS FOR ACETONITRILE (75-05-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	41.05
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	318.1
Vp (atm)	Howard (1989-1993)	1.20E-01 at 25ºC (solid)
S (mg/L)	Howard (1989-1993)	7.50E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.57E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.14E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.40E-05
K_{ow} (unitless)	log K_{ow} value cited in Karickhoff and Long (1995).	4.57E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.69E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.69E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.76E-02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-5

CHEMICAL-SPECIFIC INPUTS FOR ACETOPHENONE (98-86-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	120.50
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	293.6
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	5.20E-04 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	6.10E+03
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.03E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.73E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	4.37E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.69E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.69E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.02E+00
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-6

CHEMICAL-SPECIFIC INPUTS FOR ACROLEIN (107-02-8)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	56.06
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	185.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	3.50E-01 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	2.10E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.34E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.92E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.22E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	9.80E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.39E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.39E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.05E-01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-7

CHEMICAL-SPECIFIC INPUTS FOR ACRYLONITRILE (107-13-1)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	53.06
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	189.6
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	1.40E-01 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	7.50E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.90E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.11E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.23E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.78E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.22E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.22E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.66E-01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.10E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-8

CHEMICAL-SPECIFIC INPUTS FOR ALDRIN (309-00-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	364.93
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	377.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	2.20E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	7.84E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.02E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.43E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.40E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994f).	1.51E+06
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.87E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.87E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.65E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.95E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	4.28E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.9955

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-8a

CHEMICAL-SPECIFIC INPUTS FOR ALUMINUM (7429-90-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	26.98
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	933
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	NA
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *S* and *Vp* values are zero for all metals except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in (U.S. EPA 1996a).	2.11E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in (U.S. EPA 1996a).	2.44E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Kd_{bs} (cm^3/g)	--	ND
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile (except mercury), metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-9

CHEMICAL-SPECIFIC INPUTS FOR ANILINE (62-53-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	93.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	266.8
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	8.80E-04 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	3.60E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	2.28E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.56E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.01E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	9.55E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.23E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.23E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.17E-01
ksg (year)$^{-1}$	NC DEHNR (1997)	3.20E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-10

CHEMICAL-SPECIFIC INPUTS FOR ANTHRACENE (120-12-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	178.22
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	491.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	3.35E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	5.37E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.11E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.24E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.74E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	2.95E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.35E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.35E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.76E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.40E+02
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	5.50E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-11

CHEMICAL-SPECIFIC INPUTS FOR ANTIMONY (7440-36-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	121.75
T_m (^oK)	Budavari, O'Neil, Smith, and Heckelman (1989)	903.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	NA
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.73E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.96E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	45 at pH=6.8
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	45 at pH=6.8
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	45 at pH=6.8
ksg $(year)^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-12

CHEMICAL-SPECIFIC INPUTS FOR AROCLOR 1016 (12674-11-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	257.9
T_m (K)	--	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	9.37E-07 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.71E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.23E-04
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.69E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	5.43E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.53E+05
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.32E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.32E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.74E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.29E+02
ksg (year)$^{-1}$	Mackay, Shiu, and Ma (1992).	5.06E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table.	0.999

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-13

CHEMICAL-SPECIFIC INPUTS FOR AROCLOR 1254 (11097-69-1)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	327.0
T_m (K)	Montgomery and Welkom (1991)	283.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.16E-07 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.15E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.37E-04
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.00E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.64E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.61E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.83E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.83E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.37E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.93E+03
ksg (year)$^{-1}$	Mackay, Shiu, and Ma (1992).	5.06E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	0.993

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-14

CHEMICAL-SPECIFIC INPUTS FOR ARSENIC (7440-38-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	74.92
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1,091 at 36 atm
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.07E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.24E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	25 at pH=4.9; 29 at pH=6.8; 31 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	25 at pH=4.9; 29 at pH=6.8; 31 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	25 at pH=4.9; 29 at pH=6.8; 31 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-15

CHEMICAL-SPECIFIC INPUTS FOR ATRAZINE (1912-24-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	215.68
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	444.1
Vp (atm)	*Vp* value cited in Budavari, O'Neil, Smith, and Heckelman (1989)	3.66×10^{-10} at 25°C (solid)
S (mg/L)	*S* value cited in Howard and others 1989 - 1993	3.00E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.63E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.03E-06
K_{ow} (unitless)	log K_{ow} value cited in Karickhoff and Long (1995).	4.07E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.54E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.54E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.15E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.15E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	1.04E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.945

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-16

CHEMICAL-SPECIFIC INPUTS FOR BARIUM (7440-39-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	137.33
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	983
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.14E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.26E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-17

CHEMICAL-SPECIFIC INPUTS FOR BENZALDEHYDE (100-52-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	106.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	329.6
Vp (atm)	*Vp* value cited in NC DEHNR (1997).	1.30E-03 at 25°C (solid)
S (mg/L)	*S* value cited in NC DEHNR (1997).	3.30E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.18E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.07E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.48E-06
K_{ow} (unitless)	K_{ow} value cited in NC DEHNR (1997).	3.00E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.01E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.01E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.51E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.04E-01
ksg (year)$^{-1}$	*Ksg* value assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-18

CHEMICAL-SPECIFIC INPUTS FOR BENZENE (71-43-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	78.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	278.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.25E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.78E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.49E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.17E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.02E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	137
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	6.20E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.20E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.65E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.48E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	3.89E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-19

CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)ANTHRACENE (56-55-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	228.28
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	433
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.03E-10 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.28E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	3.62E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	2.47E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	6.21E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	4.77E+05
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	2.60E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.60E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.95E+04
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.04E+04
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.72E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	8.81E-01

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-20

CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)PYRENE (50-32-8)

(**Page 1 of 1**)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	252.3
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	452
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	6.43E-12 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.94E-03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	8.36E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database in U.S. EPA (1994d).	2.18E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database in U.S. EPA (1994d).	5.85E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.35E+06
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	9.69E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.69E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.27E+04
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.87E+04
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	4.77E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	2.65E-01

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-21

CHEMICAL-SPECIFIC INPUTS FOR BENZO(B)FLUORANTHENE (205-99-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	252.32
T_m (K)	Montgomery and Welkom (1991)	441
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.06E-10 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	4.33E-03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	6.18E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	2.28E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	5.49E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.59E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.36E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.36E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.27E+04
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.34E+04
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	4.15E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.822

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-22

CHEMICAL-SPECIFIC INPUTS FOR BENZO(K)FLUORANTHENE (207-08-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	252.32
T_m (K)	Montgomery and Welkom (1991)	490
Vp (atm)	U.S. EPA (1994b)	1.32E-12 at 25°C (solid)
S (mg/L)	U.S. EPA (1994b)	8.0E-04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	4.15E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	2.28E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	5.49E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	1.56E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.32E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.32E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.24E+04
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.33E+04
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Lyman, Reehl, and Rosenblatt (1991).	1.18E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.149

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-23

CHEMICAL-SPECIFIC INPUTS FOR BENZOIC ACID (65-85-0)

(Page 1 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	122.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	395.5
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	8.57E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.13E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.34E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.36E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.80E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	7.60E+01
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 31.98 2 31.80 3 30.13 4 19.81 5 4.81 6 0.99 7 0.55 8 0.50 9 0.50 10 0.50 11 0.50 12 0.50 13 0.50 14 0.50
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.50E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.13E-02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.20E-02

TABLE A-2-23

CHEMICAL-SPECIFIC INPUTS FOR BENZOIC ACID (65-85-0)

(Page 2 of 2)

Parameter	Reference and Explanation	Value
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited Howard (1989-1993).	1.26E+02
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-24

CHEMICAL-SPECIFIC INPUTS FOR BENZONITRILE (100-47-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	103.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	285.85
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.45E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.43E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	3.63E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.33E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.33E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.75E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.33E-01
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was assumed to be 1.0 due to a lack of data.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-25

CHEMICAL-SPECIFIC INPUTS FOR BENZYL ALCOHOL (100-51-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	108.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	288.29
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.40E-04 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	4.00E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.78E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.89E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.38E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	1.26E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.02E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.02E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.66E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.09E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-26

CHEMICAL-SPECIFIC INPUTS FOR BENZYL CHLORIDE (100-44-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	126.58
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	225.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	1.60E-03 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	4.90E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.13E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.43E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.80E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	2.00E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.83E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.83E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.62E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.53E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.09E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-27

CHEMICAL-SPECIFIC INPUTS FOR BERYLLIUM (7440-41-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	9.01
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1,560
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.39E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	5.08E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	23 at pH=4.9; 790 at pH=6.8; 1.0E+05 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	23 at pH=4.9; 790 at pH=6.8; 1.0E+05 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	23 at pH=4.9; 790 at pH=6.8; 1.0E+05 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-28

CHEMICAL-SPECIFIC INPUTS FOR ALPHA-BHC (319-84-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.0
T_m (K)	Montgomery and Welkom (1991)	432.2
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.61E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.40E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.78E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	0.0191
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.04E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994g).	6.30E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.76E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.76E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.32E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.05E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.87E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.000

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-29

CHEMICAL-SPECIFIC INPUTS FOR BETA-BHC (319-85-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.83
T_m (K)	Montgomery and Welkom (1991)	582.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	6.45E-10 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.42E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.46E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.9E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.40E-06
K_{ow} (unitless)	Geometric mean value cited in Karickoff and Long (1995).	6.81E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.14E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.14E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.60E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.56E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.04E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.999

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-30

CHEMICAL-SPECIFIC INPUTS FOR BIS(2-CHLORETHYL)ETHER (111-44-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	143.02
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	223.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.76E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.18E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.13E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.40E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.70E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	2.00E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	7.60E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.60E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.70E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.04E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-31

CHEMICAL-SPECIFIC INPUTS FOR BROMODICHLOROMETHANE (75-27-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	163.83
T_m (K)	Montgomery and Welkom (1991)	218.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.68E-02 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.97E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.17E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.98E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.06E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.06E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.38E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.38E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.03E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.15E+00
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-32

CHEMICAL-SPECIFIC INPUTS FOR BROMOFORM (75-25-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	252.77
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	280.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.82E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.21E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.16E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.41E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.03E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.24E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.26E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.26E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.45E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.04E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-33

CHEMICAL-SPECIFIC INPUTS FOR 4-BROMOPHENYL-PHENYLETHER (101-55-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	249.2
T_m (K)	Montgomery and Welkom (1991)	291.8
Vp (atm)	*Vp* value cited in Montgomery and Welkom (1991).	1.97E-06 at 25°C (liquid)
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.98E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.83E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.10E+05
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.21E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.21E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.09E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.85E+02
ksg (year)$^{-1}$	*Ksg* value wasassumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-34

CHEMICAL-SPECIFIC INPUTS FOR BUTYLBENZYLPHTHALATE (85-68-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Howard (1989-1993)	312.39
T_m (K)	Howard (1989-1993)	238.0
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.58E-08 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.58E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.91E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.65E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.17E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.59E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.37E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.37E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.03E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.50E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	9.64E-01

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-35

CHEMICAL-SPECIFIC INPUTS FOR CADMIUM (7440-43-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	112.41
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	594.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	8.16E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	9.45E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	15 at pH=4.9; 75 at pH=6.8; 4.3E+03 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	15 at pH=4.9; 75 at pH=6.8; 4.3E+03 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	15 at pH=4.9; 75 at pH=6.8; 4.3E+03 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-36

CHEMICAL-SPECIFIC INPUTS FOR CARBON DISULFIDE (75-15-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	76.14
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	161.5
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.47E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.67E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.27E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.04E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.29E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.00E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.14E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.14E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.86E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.06E+00
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-37

CHEMICAL-SPECIFIC INPUTS FOR CARBON TETRACHLORIDE (56-23-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	153.84
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	250.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.48E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.92E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.87E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.56E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.77E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.21E+02
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	1.52E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.52E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.14E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.08E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.03E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-38

CHEMICAL-SPECIFIC INPUTS FOR CHLORDANE (57-74-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	409.80
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	381.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.55E-08 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.51E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.64E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.18E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.37E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	8.66E+05
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	5.13E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.13E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.85E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.05E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.83E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.997

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-39

CHEMICAL-SPECIFIC INPUTS FOR CHLORINE (7782-50-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	71.90
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	172.1
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	--	1.10E-01
D_w (cm^2/s)	--	1.27E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Kd_{bs} (mL/g)	--	ND
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-40

CHEMICAL-SPECIFIC INPUTS FOR 4-CHLORO-3-METHYLPHENOL (59-50-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	142.58
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	328.6
Vp (atm)	U.S. EPA (1994b)	1.08E-05
S (mg/L)	U.S.EPA (1992a)	3.85E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.00E-07
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	6.96E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.06E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.26E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.71E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.71E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.78E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.48E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Lucius (1992).	1.10E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	0.9999

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-41

CHEMICAL-SPECIFIC INPUTS FOR P-CHLOROANILINE (106-47-8)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	127.57
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	345.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.09E-05 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.36E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.17E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.02E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	7.40E+01
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	K_{oc} is 41 for pH range of 4.9 to 8
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.06E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.05E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.63E+00
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due a a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-42

CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZENE (108-90-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	112.56
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	228.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.59E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.09E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.38E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.35E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.49E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	6.16E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.24E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.24E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.68E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.96E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.69E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-43

CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZILATE (510-15-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	325.20
T_m (K)	Howard (1989-1993)	309.0
Vp (atm)	Howard (1989-1993)	2.90E-09 at 25°C (solid)
S (mg/L)	Howard (1989-1993)	1.30E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.24E-08
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	1.65E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	4.72E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	2.40E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.69E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.69E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.77E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.48E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.23E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	8.62E-01

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-44

CHEMICAL-SPECIFIC INPUTS FOR CHLORODIFLUOROMETHANE (75-45-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Howard 1989-1993	86.47
T_m (K)	Howard 1989-1993	126.6
Vp (atm)	*Vp* value cited in Howard 1989-1993.	5.63 at 25°C (liquid)
S (mg/L)	Howard 1989-1993	2.90E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.68E-01
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	9.72E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.13E-05
K_{ow} (unitless)	Calculated using the log K_{ow} value cited in Howard 1989-1993.	1.20E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.83E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.83E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.38E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.93E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) OR Howard (1989-1993) OR Mackay, Shiu, and Ma (1992).	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-45

CHEMICAL-SPECIFIC INPUTS FOR CHLOROETHANE (75-00-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	64.52
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	441.8
Vp (atm)	*Vp* value cited in Lucius et al. (1992).	159.88 at 25ºC (solid)
S (mg/L)	*S* value cited in U.S. EPA (1994a)	5.74E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.80
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.27E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.53E-06
K_{ow} (unitless)	K_{ow} value calculated from log K_{ow} value cited in U.S. EPA (1995a).	1.26E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.71E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.71E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.78E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.48E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	6.72E+02
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-46

CHEMICAL-SPECIFIC INPUTS FOR CHLOROFORM (67-66-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	119.39
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	209.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.69E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.96E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.03E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.17E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.09E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	8.90E+01
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	5.30E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.30E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.98E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.12E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-47

CHEMICAL-SPECIFIC INPUTS FOR (BIS)-1,2-CHLOROISOPROPYLETHER (39638-32-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	171.07
T_m (K)	Montgomery and Welkom (1991)	369.9
Vp (atm)	Montgomery and Welkom (1991)	7.00E-03 at 25ºC (solid)
S (mg/L)	Montgomery and Welkom (1991)	1.70E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.04E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.61E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.38E-06
K_{ow} (unitless)	K_{ow} value cited in Howard (1989 - 1993).	3.80E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.46E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.46E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.09E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.82E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-48

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORONAPHTHALENE (91-58-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	162.61
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	332.6
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	1.05E-05 at 25ºC (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.20E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.43E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.64E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.24E-06
K_{ow} (unitless)	Montgomery and Welkom (1991)	1.17E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.14E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.14E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.36E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.86E+02
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-49

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLOROPHENOL (95-57-8)

(Page 1 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	128.56
T_m (K)	Montgomery and Welkom (1991)	282.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.77E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.15E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.66E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.01E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.46E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.45E+02
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 398.0 2 398.0 3 398.0 4 398.0 5 397.9 6 396.9 7 387.3 8 311.8 9 108.7 10 19.43 11 7.39 12 6.14 13 6.01 14 6.00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	3.87E+00

TABLE A-2-49

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLOROPHENOL (95-57-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties (Continued)		
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	2.90E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	1.55E+01
ksg $(year)^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-50

CHEMICAL-SPECIFIC INPUTS FOR 4-CHLOROPHENYL-PHENYLETHER (7005-72-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	204.66
T_m (K)	Montgomery and Welkom (1991)	265.1
Vp (atm)	*Vp* value cited in Montgomery and Welkom (1991).	3.55E-06 at 25°C (liquid)
S (mg/L)	*S* value cited in Montgomery and Welkom (1991).	3.30E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.20E-04
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	3.82E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.42E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	5.85E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.40E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.40E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.55E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.96E+02
ksg (year)$^{-1}$	*Ksg* value was assumed to be zero due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-51

CHEMICAL-SPECIFIC INPUTS FOR CHLOROPYRIFOS (2921-88-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	350.59
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	314.6
Vp (atm)	*Vp* value cited in Howard (1989-1993).	1.32E-03 at 25°C (solid)
S (mg/L)	*S* value cited in Howard (1989-1993).	5.00E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.26E-02
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	3.82E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.42E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	1.82E+05
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.79E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.79E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.35E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.18E+02
ksg (year)$^{-1}$	*Ksg* value was assumed to 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-52

CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM (7440-47-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	52
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	2,173.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database in U.S. EPA (1994f).	1.01E-01
D_w (cm^2/s)	D_W value was obtained from CHEMDAT8 database in U.S. EPA (1994f).	4.63E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-53

CHEMICAL-SPECIFIC INPUTS FOR HEXAVALENT CHROMIUM (18540-29-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	52
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	2,173.0
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.36E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.58E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	31 at pH=4.9; 19 at pH=6.8; 14 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	31 at pH=4.9; 19 at pH=6.8; 14 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	31 at pH=4.9; 19 at pH=6.8; 14 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-54

CHEMICAL-SPECIFIC INPUTS FOR CHRYSENE (218-01-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	228.28
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	527.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.03E-11 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.94E-03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	1.21E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	2.48E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	6.21E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.48E+05
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.97E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.97E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.23E+04
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.19E+04
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.53E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.761

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-54a

CHEMICAL-SPECIFIC INPUTS FOR COPPER (7440-50-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	63.55
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1356.15
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	NA
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *S* and *Vp* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.19E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.38E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values estimated using the MINTEQ2 geochemical speciation model.	40 at pH=4.9 10000 at pH=6.8 28,500 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for metals, as cited in U.S. EPA (1994f).	40 at pH=4.9 10000 at pH=6.8 28,500 at pH=8.0
Kd_{bs} (cm^3/g)	Kd_{bs} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for metals, as cited in U.S. EPA (1994f).	40 at pH=4.9 10000 at pH=6.8 28,500 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because metals are nonvolatile (except mercury), they are assumed to be 100 percent in the particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-55

CHEMICAL-SPECIFIC INPUTS FOR M-CRESOL (108-39-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	108.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	284.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	1.90E-04 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	2.30E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.93E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.93E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.30E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	9.10E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.78E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.78E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.58E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.91E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	8.72E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-56

CHEMICAL-SPECIFIC INPUTS FOR O-CRESOL (95-48-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	108.13
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	303.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.16E-04 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.77E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.62E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.88E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.41E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.05E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.34E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.34E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.0E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.14E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-57

CHEMICAL-SPECIFIC INPUTS FOR P-CRESOL (106-44-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	108.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	308.6
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	1.70E-04 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	2.30E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.99E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.93E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.30E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	8.70E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.61E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.61E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.46E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.84E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.79E+02
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-58

CHEMICAL-SPECIFIC INPUTS FOR CUMENE (ISOPROPYLBENZENE) (98-82-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	120.19
T_m (K)	U.S. EPA (1995b)	177
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	6.00E-03 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	5.60E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.29E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.50E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.83E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	4.10E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.31E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.31E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.98E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.72E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.16E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-59

CHEMICAL-SPECIFIC INPUTS FOR CYANIDE (57-12-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S.EPA (1992a)	26.017
T_m (K)	--	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.82E-02 at 25ºC (solid)
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	5.48E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	2.10E-05
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Kd_{bs} (cm^3/g)	--	ND
ksg (year)$^{-1}$	*Ksg* value was assumed to be zero due to a lack of data.	0.0
Fv (unitless)	*Fv* value was assumed to be 1.0 due to a lack of data.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-60

CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDD (72-54-8)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	320.05
T_m (K)	Montgomery and Welkom (1991)	380.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.14E-09 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.33E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.98E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.76E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.32E+06
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.58E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.58E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.44E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.83E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	4.34E-02
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.925

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-61

CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDE (72-55-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	319.03
T_m (K)	Montgomery and Welkom (1991)	361.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.45E-09 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.92E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.24E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.70E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.78E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.80E+06
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	8.64E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.64E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.48E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.46E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	4.34E-02
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.981

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-62

CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDT (50-29-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	354.49
T_m (K)	Montgomery and Welkom (1991)	381.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.17E-10 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.41E-03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.37E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.48E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.48E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.17E+06
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	6.78E+05
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.78E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.08E+04
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.71E+04
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	4.34E-02
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.852

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-63

CHEMICAL-SPECIFIC INPUTS FOR DI-N-BUTYL PHTHALATE (84-74-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	278.34
T_m (K)	Montgomery and Welkom (1991)	238.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.55E-08 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.08E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.43E-06
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	4.38E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	7.86E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.25E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.57E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.57E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.18E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.27E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.11E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	0.989

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-64

CHEMICAL-SPECIFIC INPUTS FOR DI-N-OCTYLPHTHALATE (117-84-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	390.56
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	248.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.88E-09 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.00E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.65E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.32E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.20E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.14E+09
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.03E+08
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.03E+06
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.78E+07
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.61E+07
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	0.9081

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-65

CHEMICAL-SPECIFIC INPUTS FOR DIAZINON (333-41-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	304.36
T_m (K)	Howard (1989-1993)	393.1
Vp (atm)	*Vp* value cited in Howard (1989-1993).	1.11E-07 at 25°C (solid)
S (mg/L)	*S* value cited in Howard (1989-1993).	6.88E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.89E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.71E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.24E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	6.46E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.33E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.33E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.96E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.31E+01
ksg (year)$^{-1}$	--	ND
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.999

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-66

CHEMICAL-SPECIFIC INPUTS FOR DIBENZ(A,H)ANTHRACENE (53-70-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	278.33
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	539.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.70E-14 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	6.70E-04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	1.12E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	1.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	6.01E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	3.53E+06
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	1.79E+06
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.79E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.34E+05
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.16E+04
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.69E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.011

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-67

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIBROMO-3-CHLOROPROPANE (96-12-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	236.36
T_m (K)	Montgomery and Welkom (1991)	279.2
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	1.0E-03 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.20E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.97E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.79E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.79E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	2.19E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.47E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.47E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.10E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.79E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-68

CHEMICAL-SPECIFIC INPUTS FOR DIBROMOCHLOROMETHANE (124-48-1)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	208.3
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	252.1
Vp (atm)	*Vp* value cited in Montgomery and Weldom (1991).	2.00E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	3.44E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.21E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.96E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.05E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994g).	1.50E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.05E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.05E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.29E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.82E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-69

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROBENZENE (95-50-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	147.01
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	256.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.79E-03 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.25E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.11E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.11E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.93E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.79E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	3.79E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.79E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.84E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.52E+01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay and others (1992).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii

TABLE A-2-70

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROBENZENE (541-73-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	147.01
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	297.86
Vp (atm)	*Vp* value cited in Howard (1989-1993).	3.03E-03 at 25°C (solid)
S (mg/L)	*S* value cited in Howard (1989-1993).	6.88E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S,* and *Vp* values that are provided in this table.	1.11E+02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.14E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.85E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	3.39E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.03E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.03E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.02E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.21E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-71

CHEMICAL-SPECIFIC INPUTS FOR 1,4-DICHLOROBENZENE (106-46-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	147.01
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	326.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.39E-03 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.30E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.80E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.14E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.85E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	2.58E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	6.16E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.16E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.62E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.46E+01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-72

CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DICHLOROBENZIDINE (91-94-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	253.13
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	405.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.89E-10 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.52E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.08E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.28E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.48E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	3.76E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.70E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.70E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.52E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.48E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. Vp value for this compound was converted to a liquid-phase value before being used in the calculations.	0.847

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-73

CHEMICAL-SPECIFIC INPUTS FOR DICHLORODIFLUOROMETHANE (75-71-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	120.92
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	115.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	6.40E+00 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	3.0E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.58E+00
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.77E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	9.00E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.44E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.85E+0
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.85E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.14E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.74E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-74

CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHANE (75-34-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	98.97
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	175.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.0E-01 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.16E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.75E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.42E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.05E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	6.20E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	5.30E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.30E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.98E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.12E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.643
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-75

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROETHANE (107-06-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	98.96
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	233.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.07E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	8.31E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.27E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.19E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.90E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.96E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.96E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.47E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.83E-01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-76

CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHYLENE (75-35-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	96.95
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	150.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.88E-01 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.0E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.55E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.53E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.09E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.32E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	6.50E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.50E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.88E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.60E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-77

CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,2-DICHLOROETHYLENE (156-59-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Howard (1989-1993)	96.94
T_m (K)	Howard (1989-1993)	192.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.30E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.94E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.51E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.36E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.13E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	9.60E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.98E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.98E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.73+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.99E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-78

CHEMICAL-SPECIFIC INPUTS FOR (TRANS)-1,2-DICHLOROETHYLENE (156-60-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	96.95
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	223.7
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	4.63E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	6.03E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.44E-03
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	8.16E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	9.75E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	9.60E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	3.80E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.80E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.85E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.52E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-79

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOL (120-83-2)

(Page 1 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	163.01
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	318.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	7.21E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	4.93E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.38E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.79E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	1.09E+03
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 159.0 2 159.0 3 159.0 4 159.0 5 158.8 6 156.8 7 139.6 8 67.31 9 12.75 10 3.50 11 2.51 12 2.41 13 2.40 14 2.40
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.40E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.05E+01

TABLE A-2-79

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOL (120-83-2)

(Page 2 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties (Continued)		
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.58E+00
ksg $(year)^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-80

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROPROPANE (78-87-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	112.99
T_m (K)	Montgomery and Welkom (1991)	172.7
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	6.66E-02 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.68E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.81E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.21E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.71E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.78E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.70E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.70E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.53E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.88E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.96E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-81

CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,3-DICHLOROPROPENE (542-75-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	110.98
T_m (K)	Montgomery and Welkom (1991)	189.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.11E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.55E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.94E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.26E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.00E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	5.60E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.70E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.70E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.03E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.08E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.24E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-82

CHEMICAL-SPECIFIC INPUTS FOR DICHLORVOS (62-73-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	220.98
T_m (K)	--	NA
Vp (atm)	*Vp* value cited in Howard (1989-1993).	6.93E-05 at 25ºC (liquid)
S (mg/L)	*S* value cited in Howard (1989-1993).	1.6E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.57E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.32E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.33E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	2.69E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.85E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.85E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.38E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.38E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	1.49E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-83

CHEMICAL-SPECIFIC INPUTS FOR DIELDRIN (60-57-1)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	380.93
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	449.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.31E-09 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.87E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.66E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.36E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	4.29E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	1.86E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.55E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.55E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.91E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.02E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	2.34E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.9860

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-84

CHEMICAL-SPECIFIC INPUTS FOR DIETHYL PHTHALATE (84-66-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	222.24
T_m (K)	Montgomery and Welkom (1991)	232.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.17E-06 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	8.80E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.48E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.56E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.35E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.73E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	8.20E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.20E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.15E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.28E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	4.52E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-85

CHEMICAL-SPECIFIC INPUTS FOR DIMETHYL PHTHALATE (131-11-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	194.19
T_m (K)	Montgomery and Welkom (1991)	273.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.17E-06 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.19E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.01E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.96E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.13E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	4.30E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.09E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.09E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.00E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.06E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-86

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DIMETHYLPHENOL (105-67-9)

(Page 1 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Moses (1978)	122.17
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	300.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	1.66E-04 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	6.25E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.24E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.84E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.69E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	2.29E+02
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 126.0 2 126.0 3 126.0 4 126.0 5 126.0 6 125.99 7 125.9 8 125.02 9 116.87 10 71.06 11 15.77 12 3.43 13 2.05 14 1.91
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.26E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.44E+00

TABLE A-2-86

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DIMETHYLPHENOL (105-67-9)

(Page 2 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties (Continued)		
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.04E+00
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-87

CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DIMETHYOXYBENZIDINE (119-90-4)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	244.28
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	410.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	3.30E-10 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	2.40E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.36E-10
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	2.38E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	5.60E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	6.46E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.65E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.65E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.74E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.46E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.877

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-88

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DINITROBENZENE (99-65-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	168.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	363
Vp (atm)	Geometric mean value cited in U.S. EPA (1994f).	4.0E-07 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994f).	5.4E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	1.25E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	3.18E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	9.15E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994f).	3.10E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.06E+01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.06E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.55E+00
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.25E-01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-89

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROPHENOL (51-28-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	184.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	385.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.52E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.8E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.82E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.73E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.06E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	3.30E+01
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 0.80 2 0.79 3 0.72 4 0.38 5 0.08 6 0.02 7 0.01 8 0.01 9 0.01 10 0.01 11 0.01 12 0.01 13 0.01 14 0.01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value calculated using the K_{oc} value that is provided in this table for a pH of 7.0.	1.0E-04 (at pH 7.0)
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	7.5E-04 (at pH 7.0)
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	4.0E-04 (at pH 7.0)

TABLE A-2-89

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROPHENOL (51-28-5)

Parameter	Reference and Explanation	Value
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.62E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.999

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-90

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROTOLUENE (121-14-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Howard (1989-1993)	182.14
T_m (K)	Howard (1989-1993)	344
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.29E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.85E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	1.46E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	3.09E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	7.86E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	9.90E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.10E+01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.10E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.83E+00
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.04E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.999

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-91

CHEMICAL-SPECIFIC INPUTS FOR 2,6-DINITROTOLUENE (606-20-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Howard (1989-1993)	182.15
T_m (K)	Howard (1989-1993)	339
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	7.47E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.05E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	1.30E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	3.11E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	7.76E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	7.70E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.19E+01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.19E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.14E+00
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.68E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-92

CHEMICAL-SPECIFIC INPUTS FOR 1,4-DIOXANE (123-91-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	88.10
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	284.9
Vp (atm)	*Vp* value cited in U.S. EPA (1995b)	5.00E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	9.00E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.89E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.20E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.05E-05
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	5.40E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.76E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.76E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.57E-02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.50E-02
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-93

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIPHENYLHYDRAZINE (122-66-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	184.24
T_m (K)	Montgomery and Welkom (1991)	401.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b)	4.74E-08 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	6.80E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.28E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.95E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.24E-06
K_{ow} (unitless)	Montgomery and Welkom (1991)	8.71E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.78E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.78E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.09E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.11E+01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.999

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-94

CHEMICAL-SPECIFIC INPUTS FOR DISULFOTON (298-04-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	274.38
T_m (K)	T_m value cited in U.S. EPA (1995b).	248
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	3.7E-07 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.6E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.12E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.50E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	5.21E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	9.55E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.80E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.80E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction oF 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.35E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.20E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.20E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.998

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-95

CHEMICAL-SPECIFIC INPUTS FOR ENDOSULFAN I (115-29-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	406.95
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	343.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.31E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	2.31E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.31E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.59E-03
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.76E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	3.02E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.04E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.04E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.53E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.16E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.78E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.9839

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-96

CHEMICAL-SPECIFIC INPUTS FOR ENDRIN (72-20-8)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	380.93
T_m (K)	U.S.EPA (1992a)	473.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a)	7.68E-10 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a)	2.46E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.19E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.07E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	5.76E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	7.79E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.08E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.08E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.11E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.32E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	3.61E+04
Fv (unitless)	--	ND

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-97

CHEMICAL-SPECIFIC INPUTS FOR EPICHLOROHYDRIN (106-89-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	92.53
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	247.5
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	2.20E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	6.60E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.08E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.13E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.78E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.22E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.22E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.66E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.88E-02
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-98

CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHACRYLATE (97-63-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	*MW* value cited in U.S. EPA (1995b)	114.14
T_m (K)	--	NA
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	2.30E-02 at 25ºC
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.90E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.38E-04
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	8.07E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	9.35E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	3.89E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.46E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.46E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.85E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.80E-01
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value cited in NC DEHNR (1997).	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-99

CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHANESULFONATE (62-50-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	124.15
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	373.0
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	3.50E-04 at 25ºC (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	4.90E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.87E-08
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.63E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.84E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.12E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.55E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	1.55E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.16E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.19E-02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.88E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-100

CHEMICAL-SPECIFIC INPUTS FOR ETHYLBENZENE (100-41-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	106.16
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	178.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.26E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.73E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.73E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.65E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.49E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.33E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.04E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.04E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.53E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.16E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	2.53E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-101

CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE DIBROMIDE (106-93-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	187.88
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	282.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	1.00E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	4.20E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.47E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.17E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.19E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	5.62E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.28E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.28E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.46E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.31E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-102

CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE OXIDE (75-21-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	44.05
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	162.1
Vp (atm)	Verschueren (1983)	1.44E+00 at 25°C (liquid)
S (mg/L)	*S* value cited in NC DEHNR (1996).	3.80E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.67E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.71E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.44E-05
K_{ow} (unitless)	Howard (1989-1993)	5.01E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.26E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.26E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.19E-02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.30E-02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.13E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-103

CHEMICAL-SPECIFIC INPUTS FOR BIS(2-ETHYLHEXYL)PHTHALATE (117-81-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	390.54
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	218.1
Vp (atm)	*Vp* value cited in U.S. EPA (1994c).	8.49E-09 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.96E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.37E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.32E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.22E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.60E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1994c).	1.11E+05
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.11E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.33E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.44E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.10E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	0.9350

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-104

CHEMICAL-SPECIFIC INPUTS FOR FLUORANTHENE (206-44-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	202.26
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	383.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.07E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.32E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.33E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.75E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.18E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	1.21E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.91E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.91E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.68E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.96E+03
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	5.75E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.992

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-105

CHEMICAL-SPECIFIC INPUTS FOR FLUORENE (86-73-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	166.22
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	389.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	8.17E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.86E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.30E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	3.63E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	7.88E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	1.47E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	7.71E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.71E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction oF 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.78E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.08E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	4.22E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.9999

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-106

CHEMICAL-SPECIFIC INPUTS FOR FORMALDEHYDE (50-00-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	30.03
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	365.1
Vp (atm)	*Vp* value cited in U.S. EPA (1994c)	5.10E+00 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	5.50E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.78E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	5.00E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.74E-05
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	2.20E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.62E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.62E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.96E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.05E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	3.61E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-107

CHEMICAL-SPECIFIC INPUTS FOR FORMIC ACID (64-18-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1995b)	46.03
T_m (K)	U.S. EPA (1995b)	282.0
Vp (atm)	*Vp* value cited in U.S. EPA (1995b)	5.40E-02 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	1.00E+06
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.49E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.22E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.71E-05
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b)	2.90E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.39E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.39E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.04E-02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.16E-02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-108

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)DIOXIN (35822-46-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	425.31
T_m (K)	U.S. EPA (1994a)	537.1
Vp (atm)	U.S. EPA (1994a)	4.22E-14 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	2.40E-06
H (atm·m^3/mol)	U.S. EPA (1994a)	7.50E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.11E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	3.89E-06
K_{ow} (unitless)	U.S. EPA (1992d)	1.58E+08
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	9.77E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.77E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.33E+06
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.91E+06
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.09E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.62E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-109

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8-HEPTACHLORODIBENZO(P)FURAN (67562-39-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	409.31
T_m (K)	U.S. EPA (1994a)	509.1
Vp (atm)	U.S. EPA (1994a)	1.75E-13 at 25ºC (solid)
S (mg/L)	U.S. EPA (1994a)	1.35E-06
H (atm·m^3/mol)	U.S. EPA (1994a)	5.30E-05
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.55E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	3.99E-06
K_{ow} (unitless)	U.S. EPA (1992d)	8.32E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	5.13E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.13E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.85E+06
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.05E+06
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	3.57E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	3.47E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-110

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,7,8,9-HEPTACHLORODIBENZO(P)FURAN (55673-89-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	409.31
T_m (K)	U.S. EPA (1994a)	494.1
Vp (atm)	U.S. EPA (1994a)	1.41E-13 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	1.40E-06
H (atm·m^3/mol)	U.S. EPA (1994a)	5.30E-05
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.55E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	3.99E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	8.32E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	5.13E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.13E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.85E+06
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.05E+06
ksg (year)$^{-1}$	*ksg* value was calculated using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	3.57E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	2.01E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-111

CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR (76-44-8)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	373.35
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	368.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.29E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.73E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.87E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.12E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.69E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.04E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	9.53E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.53E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.15E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.81E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-112

CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR EPOXIDE (1024-57-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	389.32
T_m (K)	Montgomery and Welkom (1991)	430.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	5.71E-09 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	2.68E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.29E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.32E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.23E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.62E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.18E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.18E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.38E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.87E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	4.58E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.9948

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-113

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,7,8-HEXACHLORODIBENZO(P)DIOXIN (39227-28-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	390.87
T_m (K)	U.S. EPA (1994a)	546.1
Vp (atm)	U.S. EPA (1994a)	1.33E-13 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	4.40E-06
H (atm·m^3/mol)	U.S. EPA (1994a)	1.20E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.15E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.12E-06
K_{ow} (unitless)	U.S. EPA (1992d)	6.17E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a; 1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	3.80E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.80E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.85E+06
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.52E+06
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.09E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	5.96E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-114

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,6,7,8-HEXACHLORODIBENZO(P)DIOXIN (57653-85-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	390.87
T_m (K)	U.S. EPA (1994a)	558.1
Vp (atm)	U.S. EPA (1994a)	4.74E-14 at 25ºC (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	4.40E-06
H (atm·m^3/mol)	U.S. EPA (1994a)	1.20E-05
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDD.	1.15E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.12E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	1.78E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	1.10E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.10E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.22E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.39E+05
ksg (year)$^{-1}$	*ksg* value assumed to be the same as the *ksg* value calculated for 1,2,3,4,7,8-HexaCDD. *ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.09E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	2.89E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-115

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,7,8,9-HEXACHLORODIBENZO(P)DIOXIN (19408-74-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	390.87
T_m (K)	U.S. EPA (1994a)	516.1
Vp (atm)	U.S. EPA (1994a)	6.45E-14 at 25ºC (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	4.40E-06
H (atm·m^3/mol)	U.S.EPA (1994a)	1.20E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.15E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.12E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1994a).	1.78E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a; 1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	1.10E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.10E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.22E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.39E+05
ksg (year)$^{-1}$	*ksg* value was assumed to be the same as the *ksg* value for 1,2,3,4,7,8-HexaCDD. *ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.09E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.53E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-116

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,7,8-HEXACHLORODIBENZO(P)FURAN (70648-26-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	374.87
T_m (K)	U.S. EPA (1994a)	498.6
Vp (atm)	U.S. EPA (1994a)	3.16E-13 at 25ºC (solid)
S (mg/L)	U.S. EPA (1994a)	8.25E-06
H (atm·m^3/mol)	U.S. EPA (1994a)	1.40E-05
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.62E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.23E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d)	1.78E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	1.10E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.10E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.22E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.39E+05
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	4.86E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-117

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,6,7,8-HEXACHLORODIBENZO(P)FURAN (57117-44-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	374.87
T_m (K)	U.S. EPA (1994a)	505.1
Vp (atm)	U.S. EPA (1994a)	2.89E-13 at 25ºC (solid)
S (mg/L)	U.S. EPA (1994a)	1.77E-05
H (atm·m^3/mol)	U.S. EPA (1994a)	6.10E-06
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.62E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.23E-06
K_{ow} (unitless)	Homologue groupaverage value obtained from U.S. EPA (1992d)	1.78E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	1.10E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.10E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.22E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.39E+05
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	5.15E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-118

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,7,8,9-HEXACHLORODIBENZO(P)FURAN (72918-21-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	374.87
T_m (K)	U.S. EPA (1994a)	519.1
Vp (atm)	U.S. EPA (1994a)	2.37E-13 at 25ºC (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	1.30E-05
H (atm·m^3/mol)	U.S. EPA (1994a)	1.00E-05
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.62E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.23E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	1.78E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	1.10E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.10E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.22E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.39E+05
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.5759

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-119

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6,7,8-HEXACHLORODIBENZO(P)FURAN (60851-34-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	374.87
T_m (K)	U.S. EPA (1994a)	512.1
Vp (atm)	U.S. EPA (1994a)	2.63E-13 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	1.30E-05
H (atm·m^3/mol)	U.S. EPA (1994a)	1.00E-05
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.62E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.23E-06
K_{ow} (unitless)	Homologue group average value obtained from U.S. EPA (1992d).	1.78E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	1.10E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.10E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.22E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.39E+05
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	5.47E-02

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-120

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLORO-1,3-BUTADIENE (PERCHLOROBUTADIENE) (87-68-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	260.76
T_m (K)	Montgomery and Welkom (1991)	252.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.33E-04 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.54E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.39E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.73E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.33E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.38E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.94E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.94E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.20E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.77E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-121

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROBENZENE (118-74-1)

(**Page 1 of 1**)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	284.8
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	504.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.62E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	8.62E-03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	5.35E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	1.41E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	7.84E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	3.18E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	8.00E+04
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.00E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.00E+03
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.20E+03
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.21E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-122

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOPENTADIENE (77-47-4)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	272.77
T_m (K)	Montgomery and Welkom (1991)	264.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	9.63E-05 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.53E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.72E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.61E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.21E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	8.07E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.51E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.51E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.13E+2
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.80E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-123

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROETHANE (67-72-1)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, Heckelman (1989)	236.74
T_m (K)	Montgomery and Welkom (1991)	459.7
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	6.21E-04 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.08E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.60E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.77E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.88E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	9.66E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.82E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.82E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.36E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.27E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-124

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPHENE (70-30-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith and Heckleman (1989)	406.92
T_m (K)	Budavari, O'Neil, Smith and Heckleman (1989)	437.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	3.60E-15 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	3.0E-03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.88E-10
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	3.46E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.01E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	3.47E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.08E+06
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.08E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.08E+04
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.31E+04
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.71E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.4E-04

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-125

CHEMICAL-SPECIFIC INPUTS FOR HYDROGEN CHLORIDE (7647-01-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	36.47
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	158.9
Vp (atm)	U.S. EPA (1994b)	4.6E+01 (liquid)
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.73E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	2.00E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Kd_{bs} (mL/g)	--	ND
ksg (year)$^{-1}$	--	ND
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-126

CHEMICAL-SPECIFIC INPUTS FOR INDENO(1,2,3-CD)PYRENE (193-39-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	276.34
T_m (K)	Montgomery and Welkom (1991)	435
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.88E-13 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.07E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	4.86E-09
D_a (cm^2/s)	D_a value was obtained from WATER8 model database U.S. EPA (1995d)	1.90E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database U.S. EPA (1995d)	5.66E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	8.22E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.11E+06
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.11E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.08E+05
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.64E+05
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.47E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.007

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-127

CHEMICAL-SPECIFIC INPUTS FOR ISOPHORONE (78-59-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	138.21
T_m (K)	Montgomery and Welkom (1991)	265.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	5.38E-04 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.20E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.20E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.22E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.50E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.00E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.99E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.99E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.25E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.20E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-128

CHEMICAL-SPECIFIC INPUTS FOR LEAD (7439-92-1)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	207.2
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	600.5
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	5.43E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	6.28E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from Baes, Sharp, Sjoreen, and Shor (1984), which states that several factors, such as experimental methods and soil type, could influence partitioning or Kd_s values. Baes, Sharp, Sjoreen, and Shor (1984) compares values between various literature sources and provide this value, which is based on its best judgment.	9.00E+02
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	9.00E+02
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	9.00E+02
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-129

CHEMICAL-SPECIFIC INPUTS FOR MALATHIONE (121-75-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	330.36
T_m (K)	Montgomery and Welkom (1991)	276
Vp (atm)	*Vp* value cited in Howard (1989-1993).	1.04E-08 at 25°C (liquid)
S (mg/L)	*S* value cited in Howard (1989-1993).	1.43E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.40E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.47E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.29E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	2.29E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.81E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.81E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.36E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.92E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	0.946

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-130

CHEMICAL-SPECIFIC INPUTS FOR MERCURIC CHLORIDE (7487-94-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	271.52
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	550.1
Vp (atm)	U.S. EPA (1996a)	1.20E-04
S (mg/L)	Budavari, O'Neil, Smith, and Heckelman (1989)	6.90E+04
H (atm·m^3/mol)	U.S. EPA (1997g)	7.1E-10
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1997g).	4.53E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	5.25E-06
K_{ow} (unitless)	U.S. EPA (1996a)	6.10E-01
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	U.S. EPA (1997g)	5.80E+04
Kd_{sw} (L/Kg)	U.S. EPA (1997g)	1.00E+05
Kd_{bs} (mL/g)	U.S. EPA (1997g)	5.00E+04
ksg (year)$^{-1}$	U.S. EPA (1996a)	0.0
Fv (unitless)	Estimated based on discussions concerning divalent mercury provided in U.S. EPA (1996a).	0.85

Note:
NA = Not Applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-131

CHEMICAL-SPECIFIC INPUTS FOR MERCURY (7439-97-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	200.59
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	234.23
Vp (atm)	Budavari, O'Neil, Smith, and Heckelman (1989)	2.63E-06 at 25°C
S (mg/L)	Budavari, O'Neil, Smith, and Heckelman (1989)	5.62E-02
H (atm·m^3/mol)	U.S. EPA (1997g)	7.1E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database in U.S. EPA (1994d). CHEMDAT8 uses correlations with density and molecular weight to calculate D_a values. A density value of 13.546 g/cc for mercury was used.	1.09E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database in U.S. EPA (1994d). CHEMDAT8 uses correlations with density and molecular weight to calculate D_w values. A density value of 13.546 g/cc for mercury was used.	3.01E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	U.S.EPA (1997g)	1.00E+03
Kd_{sw} (L/Kg)	U.S.EPA (1997g)	1.00E+03
Kd_{bs} (mL/g)	U.S.EPA (1997g)	3.00E+03
ksg (yr)$^{-1}$	U.S. EPA (1996a)	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not available
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-132

CHEMICAL-SPECIFIC INPUTS FOR METHACRYLONITRILE (126-98-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	67.09
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	237.3
Vp (atm)	*Vp* value cited in U.S. EPA (1995b)	8.90E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	2.50E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.39E-04
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.15E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.33E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	3.47E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.74E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.74E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.80E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.49E-01
ksg (year)$^{-1}$	*Ksg* value was assumed to be zero due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-133

CHEMICAL-SPECIFIC INPUTS FOR METHANOL (67-56-1)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	32.04
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	175.3
Vp (atm)	*Vp* value cited in Montgomery and Welkom (1991)	1.30E-01 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	2.90E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.44E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	4.58E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.64E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	1.95E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.96E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.96E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.97E-02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.58E-02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-134

CHEMICAL-SPECIFIC INPUTS FOR METHOXYCHLOR (72-43-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	345.65
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	351.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.62E-09 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	8.84E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.33E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.30E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.59E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	3.36E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	8.00E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.00E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.00E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.20E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	6.93E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.901

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-135

CHEMICAL-SPECIFIC INPUTS FOR METHYL ACETATE (79-20-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	74.08
T_m (K)	Montgomery and Welkom (1991)	175.1
Vp (atm)	*Vp* value cited in Howard (1989-1993).	2.84E-01 at 25°C (liquid)
S (mg/L)	*S* value cited in Howard (1989-1993).	2.44E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.64E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.23E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-05
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	2.90E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.25E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.25E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.44E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.30E-01
ksg (year)$^{-1}$	*Ksg* value assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-136

CHEMICAL-SPECIFIC INPUTS FOR METHYL BROMIDE (74-83-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith and Heckelman (1989)	94.95
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	179.44
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.16E+00 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.45E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.41E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.28E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.21E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.30E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	9.00E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.00E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.75E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.60E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

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Note
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-137

CHEMICAL-SPECIFIC INPUTS FOR METHYL CHLORIDE (74-87-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	50.49
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	176.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.68E+00 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	6.34E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.52E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.13E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.39E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	8.00E+00
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	6.00E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.00E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.50E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.40E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boehling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-138

CHEMICAL-SPECIFIC INPUTS FOR METHYL ETHYL KETONE (78-93-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	72.10
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	187.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	1.20E-01 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	2.40E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.61E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.35E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.03E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.91E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.34E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.34E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.76E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.36E-02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-139

CHEMICAL-SPECIFIC INPUTS FOR METHYL ISOBUTYL KETONE (108-10-1)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	100.16
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	188.4
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	2.50E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	2.00E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.25E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.59E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.36E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.55E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.20E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.20E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.00E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.80E-01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-140

CHEMICAL-SPECIFIC INPUTS FOR METHYL MERCURY (22967-92-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1997g)	216.0
T_m (^oK)	--	ND
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	U.S. EPA (1997g)	4.7E-07
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1997g).	5.28E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	6.11E-06
K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (mL/g)	U.S. EPA (1997g)	7.00E+03
Kd_{sw} (L/Kg)	U.S. EPA (1997g)	1.00E+05
Kd_{bs} (mL/g)	U.S. EPA (1997g)	3.00E+03
ksg $(year)^{-1}$	U.S. EPA (1996a)	0.0
Fv (unitless)	Based on discussions provided in U.S. EPA (1996a), methyl mercury does not exist in the air/vapor phase.	0.0

Note:
NA = Not Applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-141

CHEMICAL-SPECIFIC INPUTS FOR METHYL PARATHION (298-00-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	263.23
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	310.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	1.30E-08 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	5.00E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.84E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.87E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.43E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	7.20E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.40E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.40E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.80E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.59E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.03E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.966

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-142

CHEMICAL-SPECIFIC INPUTS FOR METHYLENE BROMIDE (74-95-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	173.86
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	220.4
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	2.20E+00 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.45E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.64E-02
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	6.10E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.06E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	4.17E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.60E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.60E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.95E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.04E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-143

CHEMICAL-SPECIFIC INPUTS FOR METHYLENE CHLORIDE (75-09-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	84.94
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	178.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.87E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.74E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.38E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	8.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	1.25E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.80E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.00E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.00E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.50E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.00E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-144

CHEMICAL-SPECIFIC INPUTS FOR NAPHTHALENE (91-20-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	128.16
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	353.3
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.17E-04 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.11E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.82E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	5.26E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	8.92E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.36E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.19E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.19E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.93E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.76E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	5.27E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-145

NICKEL (7440-02-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	58.69
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1,828
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.26E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.46E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	16 at pH=4.9; 65 at pH=6.8; 1,900 at pH=8.0;
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	16 at pH=4.9; 65 at pH=6.8; 1,900 at pH=8.0;
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	16 at pH=4.9; 65 at pH=6.8; 1,900 at pH=8.0;
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-146

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROANILINE (88-74-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	138.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	342.1
Vp (atm)	*Vp* value cited in Montgomery and Welcom (1991).	1.07E-05 at 25°C (solid)
S (mg/L)	*S* value cited in Montgomery and Welcom (1991).	1.26E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.17E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.29E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.81E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	7.08E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.93E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.93E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.95E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.57E+00
ksg (year)$^{-1}$	*Ksg* value wasassumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-147

CHEMICAL-SPECIFIC INPUTS FOR 3-NITROANILINE (99-09-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	138.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	387.1
Vp (atm)	--	1.07E-05 at 25°C (solid)
S (mg/L)	*S* value cited in Montgomery and Welcom (1991)	8.90E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant.	1.65E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.11E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.23E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	2.34E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.66E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.66E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.24E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.62E-01
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was assumed to be 1.0 due to a lack of data.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-148

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROANILINE (100-01-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	138.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	419.10
Vp (atm)	--	ND
S (mg/L)	*S* value cited in Montgomery and Welcom (1991)	1.07E-05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant.	1.65E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.31E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.75E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	2.46E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.72E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.72E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.29E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.89E-01
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was assumed to be 1.0 due to a lack of data.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-149

CHEMICAL-SPECIFIC INPUTS FOR NITROBENZENE (98-95-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	123.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	279.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	3.21E-04 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.92E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	2.06E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	5.43E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	9.43E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	6.80E+01
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.19E+02
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.19E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.93E+00
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.76E+004
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.28E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the liquid-phase *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-150

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPHENOL (88-75-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	139.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	317.1
Vp (atm)	*Vp* value cited in Howard (1989-1993).	2.63E-04 at 25°C (solid)
S (mg/L)	*S* value cited in Howard (1989-1993).	2.50E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S,* and *Vp* values that are provided in this table.	1.46E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.44E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.19E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	6.17E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.53E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.53E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.65E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.41E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-151

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROPHENOL (100-02-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	139.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	386.1
Vp (atm)	*Vp* value cited in Howard (1989-1993).	1.32E-06 at 25°C (solid)
S (mg/L)	*S* value cited in Howard (1989-1993).	2.50E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.32E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.30E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.61E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	8.13E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.37E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.37E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.28E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.75E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.09E+02
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-152

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSO-DI-N-BUTYLAMINE (924-16-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	*MW* value cited in U.S. EPA (1995b)	158.20
T_m (K)	--	NA
Vp (atm)	*Vp* value cited in U.S. EPA (1995b)	3.80E-04 at 25°C
S (mg/L)	*S* value cited in U.S. EPA (1995b)	1.10E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.47E-05
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	6.50E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.52E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	2.57E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.07E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.07E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.05E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.29E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.44E+00
Fv (unitless)	*Fv* value cited in NC DEHNR (1997).	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-153

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPHENYLAMINE (86-30-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	198.23
T_m (K)	Montgomery and Welkom (1991)	339.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.32E-04 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	3.74E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.99E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.12E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.35E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.06E+03
K_{oc} (mL/g)	Estimated value was obtained from U.S. EPA (1994c).	3.27E+02, for pH range of 4.9 to 8.0
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.27E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.45E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.31E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.44E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-154

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPROPYLAMINE (621-64-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	130.19
T_m (K)	--	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.63E-03 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.46E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.13E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.67E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.75E-06
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	2.40E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.70E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.70E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.28E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.80E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-155

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)DIOXIN (3268-87-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	460.76
T_m (K)	U.S. EPA (1994a)	598.1
Vp (atm)	U.S. EPA (1994a)	1.09E-15 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	7.40E-08
H (atm·m^3/mol)	U.S. EPA (1994a)	7.00E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.06E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	3.69E-07
K_{ow} (unitless)	U.S. EPA (1994a)	3.89E+07
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a; 1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	2.40E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.40E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.80E+06
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.60E+05
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.09E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.0017

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-156

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,4,6,7,8,9-OCTACHLORODIBENZO(P)FURAN (39001-02-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	444.76
T_m (K)	U.S. EPA (1994a)	531.1
Vp (atm)	U.S. EPA (1994a)	4.93E-15 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	1.20E-06
H (atm·m^3/mol)	U.S.EPA (1994a)	1.90E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.48E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	3.78E-06
K_{ow} (unitless)	U.S. EPA (1994a)	6.03E+08
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	3.72E+08
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.72E+06
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.79E+07
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.49E+07
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.10E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.67E-03

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-157

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,7,8-PENTACHLORODIBENZO(P)DIOXIN (40321-76-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	356.42
T_m (K)	U.S. EPA (1994a)	513.1
Vp (atm)	U.S. EPA (1994a)	1.25E-12 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	1.20E-04
H (atm·m^3/mol)	U.S. EPA (1994a)	2.60E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.21E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.38E-06
K_{ow} (unitless)	U.S. EPA (1992d)	4.37E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	2.69E+06
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.69E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.02E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.08E+05
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	2.19E-01

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-158

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3,7,8-PENTACHLORODIBENZO(P)FURAN (57117-41-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	340.42
T_m (K)	U.S. EPA (1994a)	498.1
Vp (atm)	U.S. EPA (1994a)	3.58E-12 at 25°C (solid)
S (mg/L)	Homologue group average value obtained from U.S. EPA (1994a).	2.40E-04
H (atm·m^3/mol)	U.S. EPA (1994a)	6.20E-06
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.70E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.51E-06
K_{ow} (unitless)	U.S. EPA (1992d)	6.17E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	3.80E+06
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.80E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.85E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.52E+05
ksg (year)$^{-1}$	*ksg* value assumed to be the same as the *ksg* value calculated for 2,3,4,7,8-PentaCDF. *ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	3.57E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	3.64E-01

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-159

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,7,8-PENTACHLORODIBENZO(P)FURAN (57117-31-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	340.42
T_m (K)	U.S. EPA (1994a)	469.1
Vp (atm)	U.S. EPA (1994a)	4.33E-12 at 25ºC (solid)
S (mg/L)	U.S. EPA (1994a)	2.36E-04
H (atm·m^3/mol)	U.S. EPA (1994a)	6.20E-06
D_a (cm^2/s)	D_a value was calculated by using Equation A-3-2. Recommended value was calculated by using the *MW* and D_a values that are provided in the tables in Appendix A-2 for 2,3,7,8-TCDF.	1.70E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.51E-06
K_{ow} (unitless)	U.S. EPA (1992d)	8.32E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a) and U.S. EPA (1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	5.13E+06
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.13E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.85E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.05E+05
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	3.57E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	2.63E-01

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-160

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROBENZENE (608-93-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	250.34
T_m (K)	Montgomery and Welkom (1991)	358.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994f)	3.10E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994f)	3.20E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.43E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.86E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.34E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	1.22E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	3.21E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.21E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.41E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.29E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.33E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-161

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	295.36
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	417.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994f). U.S. EPA (1994c) cites value from Howard (1989-1993)	3.1E-06 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994f); U.S. EPA (1994c) cites value from Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.20E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt, (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	2.86E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	1.87E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	5.0E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994f).	4.37E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.89E+03
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.89E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.42E+02
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.36E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.62E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-162

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

(**Page 1 of 2)**

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	266.35
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	463
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	7.11E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.34E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	1.41E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	1.56E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	8.01E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.20E+05
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 19,949 2 19,918 3 19,604 4 16,942 5 7,333 6 1,417 7 504.9 8 408.7 9 399.1 10 398.1 11 398.0 12 398.0 13 398.0 14 398.0
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	pH / K_{oc} 1 199.5 2 199.2 3 196.0 4 169.4 5 73.33 6 14.17 7 5.05 8 4.09 9 3.99 10 3.98 11 3.98 12 3.98 13 3.98 14 3.98

TABLE A-2-162

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

(**Page 2 of 2**)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties (Continued)		
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	pH / K_{oc} 1 / 1,496 2 / 1,494 3 / 1,470 4 / 1,271 5 / 550.0 6 / 106.2 7 / 37.87 8 / 30.66 9 / 29.93 10 / 29.86 11 / 29.85 12 / 29.85 13 / 29.85 14 / 29.85
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	pH / K_{oc} 1 / 798.0 2 / 796.7 3 / 784.1 4 / 677.7 5 / 293.3 6 / 56.67 7 / 20.20 8 / 16.35 9 / 15.96 10 / 15.92 11 / 15.92 12 / 15.92 13 / 15.92 14 / 15.92
ksg $(year)^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.42E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in of LIST OF VARIABLES on page A-2-ii.

TABLE A-2-163

CHEMICAL-SPECIFIC INPUTS FOR PHENANTHRENE (85-01-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	178.22
T_m (K)	Montgomery and Welkom (1991)	371.1
Vp (atm)	Geometric mean value calculated from values cited in Montgomery and Welkom (1991).	1.35E-03 at 25ºC (solid)
S (mg/L)	*S* value cited in Lucius et al. (1992).	1.28E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.88E-01
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.33E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.47E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	3.55E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.09E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.09E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.57E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.35E+02
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.26E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-164

CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

(Page 1 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	94.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	314.0
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.74E-04 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	9.08E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.95E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.27E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.03E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	3.00E+01
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 22.0 2 22.0 3 22.0 4 22.0 5 22.0 6 22.0 7 22.0 8 21.8 9 20.0 10 11.2 11 2.27 12 0.51 13 0.32 14 0.30
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.20E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.65E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.79E-01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	2.53E+01

TABLE A-2-164

CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

Parameter	Reference and Explanation	Value
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-165

CHEMICAL-SPECIFIC INPUTS FOR PHORATE (298-02-2)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	260.4
T_m (K)	--	ND
Vp (atm)	*Vp* value cited in Montgomery and Welkom (1991).	1.70E-06 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	3.80E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.16E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.05E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.88E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	6.46E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.33E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.33E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.96E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.31E+01
ksg (year)$^{-1}$	*Ksg value* was assumed to be zero due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-166

CHEMICAL-SPECIFIC INPUTS FOR PHTHALIC ANHYDRIDE (85-44-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	148.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	403.9
Vp (atm)	Howard (1989-1993)	2.63E-07 at 25°C (solid)
S (mg/L)	Howard (1989-1993)	6.20E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.28E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.04E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.97E-06
K_{ow} (unitless)	NC DEHNR (1997)	2.5E-01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.10E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.10E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.57E-02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.40E-03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.35E+04
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-167

CHEMICAL-SPECIFIC INPUTS FOR PRONAMIDE (23950-58-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	256.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	428.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b)	5.30E-07 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	1.50E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.05E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.71E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	5.45E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	3.24E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.74E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.74E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.81E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.10E+01
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-168

CHEMICAL-SPECIFIC INPUTS FOR PYRENE (129-00-0)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	202.24
T_m (K)	Montgomery and Welkom (1991)	429.1
Vp (atm)	*Vp* value cited in U.S. EPA (1994c).	5.59E-09 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1994c).	1.37E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.25E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.72E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.14E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.00E+05
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	6.80E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.80E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.10E+03
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.72E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992)	1.33E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.9946

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-169

CHEMICAL-SPECIFIC INPUTS FOR PYRIDINE (110-86-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	79.10
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	231.5
Vp (atm)	*Vp* value cited in U.S. EPA (1995b)	2.60E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	3.00E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.86E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.08E-05
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	4.68E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.72E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.72E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.54E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.89E-01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-170

CHEMICAL-SPECIFIC INPUTS FOR RONNEL (299-84-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	321.57
T_m (K)	Montgomery and Welkom (1991)	314.1
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.05E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.69E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	1.17E+05
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.28E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.28E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.56E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.10E+02
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was assumed to be 1.0 due to a lack of data.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-171

CHEMICAL-SPECIFIC INPUTS FOR SAFROLE (94-59-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	162.18
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	284.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	1.10E-04 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.50E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.19E-05
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	4.06E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	7.16E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	4.57E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.68E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.68E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.26E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.73E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-172

CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	78.96
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	490.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.03E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.20E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)		NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-173

CHEMICAL-SPECIFIC INPUTS FOR SILVER (7440-22-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	107.87
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1,233.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	8.38E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	9.71E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-174

CHEMICAL-SPECIFIC INPUTS FOR STRYCHNINE (57-24-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	334.40
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	541.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	2.20E-13 at 25°C (solid)
S (mg/L)	Montgomery and Welkom (1991)	1.50E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.90E-13
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.38E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.58E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	8.51E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.53E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.53E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.40E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.81E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	9.03E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using S, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	0.086

Note:
NA = Note applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-175

CHEMICAL-SPECIFIC INPUTS FOR STYRENE (100-42-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	104.14
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	242.5
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	8.21E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.57E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.33E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.73E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.77E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	8.49E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	9.12E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.12E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.84E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.65E+01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-176

CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8-TETRACHLORODIBENZO(P)DIOXIN (1746-01-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	321.98
T_m (K)	U.S. EPA (1994a)	578.1
Vp (atm)	U.S. EPA (1994a)	9.74E-13 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	1.93E-05
H (atm·m^3/mol)	U.S. EPA (1994a)	1.60E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.27E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.81E-06
K_{ow} (unitless)	U.S. EPA (1994a)	4.37E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a; 1994b). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	2.69E+06
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.69E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.02E+05
Kd_{bs} (mL/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.08E+05
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	4.29E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.4901

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-177

CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8-TETRACHLORODIBENZO(P)FURAN (51207-31-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	305.98
T_m (K)	U.S. EPA (1994a)	500.1
Vp (atm)	U.S. EPA (1994a)	1.17E-11 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	4.19E-04
H (atm·m^3/mol)	U.S. EPA (1994a).	8.60E-06
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	1.79E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.85E-06
K_{ow} (unitless)	U.S. EPA (1992d)	3.39E+06
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a; 1994c). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	2.09E+06
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.09E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.57E+05
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.36E+04
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	3.57E-01
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of Fv was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid phase value before being used in the calculations.	0.6634

Note:
NA = Not Applicable
ND = No Data Available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-178

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4,5-TETRACHLOROBENZENE (95-94-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	215.89
T_m (K)	Montgomery and Welkom (1991)	411.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	7.1E-06 at 25ºC (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.30E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.18E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.11E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.75E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	4.36E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.89E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.89E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.42E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	2.36E+02
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-179

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1,2-TETRACHLOROETHANE (630-20-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	167.85
T_m (K)	Montgomery and Welkom (1991)	230.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b)	1.60E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b)	1.10E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.44E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.15E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.30E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	4.27E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.59E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.59E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.20E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.37E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	5.75E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-180

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2,2-TETRACHLOROETHANE (79-34-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	167.86
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	229.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	6.80E-03 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.07E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.72E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.16E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.26E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	4.40E+04
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	7.90E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.90E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.93E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.16E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	5.75E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-181

CHEMICAL-SPECIFIC INPUTS FOR TETRACHLOROETHYLENE (127-18-4)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	165.85
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	251.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	2.42E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	2.32E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.73E-02
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	7.20E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	8.20E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	3.51E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.65E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.65E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.99E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.06E+01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.03E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-182

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

(Page 1 of 2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1995b)	231.89
T_m (K)	U.S. EPA (1995b)	343.0
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	6.60E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.00E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from, Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.53E-05
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	2.55E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	5.78E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.0E+04
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 / 6,190 2 / 6,188 3 / 6,166 4 / 5,956 5 / 4,456 6 / 1,323 7 / 249.2 8 / 115.3 9 / 101.6 10 / 100.2 11 / 100.0 12 / 100.0 13 / 100.0 14 / 100.0
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table for a *pH* of 7.0.	2.49
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	18.69
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	9.97
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41

TABLE A-2-182

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

Parameter	Reference and Explanation	Value
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-183

CHEMICAL-SPECIFIC INPUTS FOR TETRAHYDROFURAN (109-99-9)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	72.1
T_m (K)	Montgomery and Welkom (1991)	164.6
Vp (atm)	*Vp* value cited in Budavari, O'Neil, Smith, and Heckleman (1989).	2.14E-01 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1994b).	1.00E+06
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.54E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.31E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.07E-05
K_{ow} (unitless)	Value cited in Karickoff and Long (1995).	2.80E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.16E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.16E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.37E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.26E-01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard (1989-1993).	4.43E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-184

CHEMICAL-SPECIFIC INPUTS FOR THALLIUM (7440-28-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	204.38
T_m (^oK)	Budavari, O'Neil, Smith, and Heckelman (1989)	576.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	5.48E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	6.34E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
ksg $(year)^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-185

CHEMICAL-SPECIFIC INPUTS FOR TOLUENE (108-88-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	92.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	178.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	3.71E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	5.58E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.13E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.72E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.23E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	4.65E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.40E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.40E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.05E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.60E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	1.15E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-186

CHEMICAL-SPECIFIC INPUTS FOR O-TOLUIDINE (95-53-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	107.15
T_m (K)	Montgomery and Welkom (1991)	258.4
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	3.94E-04 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.74E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.43E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.14E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.12E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	2.19E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.57E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.57E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.18E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.28E-01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-187

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROBENZENE (87-61-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	181.46
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	325.7
Vp (atm)	Geometric mean value calculated from values cited in Mackay, Shiu, and Ma (1991).	3.20E-04 at 25°C (solid)
S (mg/L)	Geometric mean value calculated from values cited in Mackay, Shiu, and Ma (1991).	2.05E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S,* and *Vp* values that are provided in this table.	2.84E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.02E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.15E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.11E+04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.02E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.02E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.52E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	8.10E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-188

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4-TRICHLOROBENZENE (120-82-1)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	181.46
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	290.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	4.42E-04 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	3.07E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.61E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.23E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	9.73E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.66E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.66E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.24E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.64E+01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991) and Mackay, Shiu, and Ma (1992).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-189

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1-TRICHLOROETHANE (71-55-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	133.42
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	242.7
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.63E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.17E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.86E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.66E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.56E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c)	2.64E+02
K_{oc} (mL/g)	Geometric mean value cited in U.S. EPA (1996b)	1.35E+05
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.35E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.01E+04
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.40E+03
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.26E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-190

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLOROETHANE (79-00-5)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	133.42
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	238.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.31E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.40E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.00E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.51E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.0E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.25E+02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	7.50E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.50E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.63E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.00E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	6.93E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-191

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROETHYLENE (79-01-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	131.40
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	188.3
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	9.48E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.18E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.06E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.65E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.94E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	2.71E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.40E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.40E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.05E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.76E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	0.703
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-192

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROFLUOROMETHANE (75-69-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	137.38
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	162.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	1.10E+00 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.10E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.37E-01
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.27E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.0E-05
K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995b).	3.40E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.34E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.34E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.00E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	5.34E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.03E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-193

CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOL (95-95-4)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	197.46
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	340.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.15E-05 at 25ºC (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.53E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.64E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.91E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.03E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	7.41E+03
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 2,380 2 2,380 3 2,380 4 2,377 5 2,353 6 2,139 7 1,127 8 223.7 9 56.14 10 37.94
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value calculated using the K_{oc} value that is provided in this table for a pH of 7.0.	1.13E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	8.45E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Kd_{bs} value calculated using the K_{oc} value that is provided in this table for a pH of 7.0.	4.51E+01
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	0.367
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-194

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	197.46
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	342.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.55E-05 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.53E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.06E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.62E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.08E-06
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.15E+03
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 / 1,070 2 / 1,070 3 / 1,069 4 / 1,063 5 / 1,006 6 / 670.8 7 / 226.2 8 / 120.4 9 / 108.4 10 / 107.1
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Kd_s value calculated using the K_{oc} value that is provided in this table for a pH of 7.0.	2.26E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	1.70E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	9.05E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.61E+00

TABLE A-2-194

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

Parameter	Reference and Explanation	Value
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-195

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROPROPANE (96-18-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	147.43
T_m (K)	Montgomery and Welkom (1991)	258.4
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	4.90E-03 at 25ºC (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.90E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.80E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.99E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.24E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.78E+02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.05E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.10E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.04E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	3.22E+00
ksg (year)$^{-1}$	*ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	7.03E-01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-196

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRIMETHYLBENZENE (108-67-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	120.19
T_m (K)	Montgomery and Welkom (1991)	287.9
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	1.30E-03 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	2.00E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.81E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.48E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.86E-06
K_{ow} (unitless)	K_{ow} value cited in Howard (1989-1993).	2.63E+03
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.67E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.67E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.25E+02
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	6.69E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Mackay, Shiu, and Ma (1992).	3.16E+01
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-197

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRINITROBENZENE (99-35-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	213.11
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	395.6
Vp (atm)	*Vp* value cited in U.S. EPA (1995b).	1.30E-07 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995b).	3.20E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.66E-08
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	2.84E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	6.08E-06
K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	1.51E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.18E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.18E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.84E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.72E-01
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using *S*, T_m, and *Vp* values that are provided in this table. *Vp* value for this compound was converted to a liquid-phase value before being used in the calculations.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-198

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6 -TRINITROTOLUENE (118-96-7)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	227.13
T_m (K)	Montgomery and Welkom (1991)	353.2
Vp (atm)	Value cited in U.S. EPA (1994b).	2.63E-07
S (mg/L)	Value cited in U.S. EPA (1994b).	1.30E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.59E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.62E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.85E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	3.98E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.51E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.51E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.88E+00
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.00E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991)	1.41E+00
Fv (unitless)	*Fv* value was assumed to be 1.0 due to a lack of data.	0.9980

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-199

CHEMICAL-SPECIFIC INPUTS FOR VINYL ACETATE (108-05-4)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	86.09
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	180.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.43E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.24E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.50E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.94E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.00E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	5.00E+00
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.97E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.97E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.73E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.99E-01
ksg (year)$^{-1}$	*Ksg* value was assumed to be 0 due to a lack of data.	0.0
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA= Not applicable
ND= No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-200

CHEMICAL-SPECIFIC INPUTS FOR VINYL CHLORIDE (75-01-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	62.50
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	119.3
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.68E+00 at 25ºC (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.30E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.15E-01
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.58E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.19E-05
K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.40E+01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.11E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.11E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.32E-01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies depending on the fraction of organic fraction in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	4.44E-01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	1.41E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in this table.	1.0

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-201

CHEMICAL-SPECIFIC INPUTS FOR *M*-XYLENE (108-38-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	106.16
T_m (K)	Montgomery and Welkom (1991)	225.7
Vp (atm)	*Vp* value cited in U.S. EPA (1994c).	1.06E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1994c).	1.86E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.05E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.49E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	1.59E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.96E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.96E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.47E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	7.84E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.000

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-202

CHEMICAL-SPECIFIC INPUTS FOR *O*-XYLENE (95-47-6)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	106.16
T_m (K)	Montgomery and Welkom (1991)	248.1
Vp (atm)	*Vp* value cited in U.S. EPA (1994c).	1.06E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1994c).	1.86E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.05E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.44E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	1.35E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.41E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.41E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.81E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	9.64E+00
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using the equation cited in Junge (1977). Recommended value of *Fv* was calculated by using the *Vp* value that is provided in the table.	1.000

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-203

CHEMICAL-SPECIFIC INPUTS FOR *P*-XYLENE (106-42-3)

(Page 1 of 1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	106.16
T_m (K)	Montgomery and Welkom (1991)	286.1
Vp (atm)	*Vp* value cited in U.S. EPA (1994c).	1.06E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1994c).	1.86E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.05E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.61E+02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.50E-06
K_{ow} (unitless)	Recommended K_{ow} value cited in Karickhoff and Long (1995).	1.48E+03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	3.11E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.11E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.33E+01
Kd_{bs} (cm^3/g)	Kd_{bs} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993d) for an assumed organic carbon fraction of 0.04 in bottom sediment. Measured organic carbon in bottom sediment, specific to site conditions, should be used to calculate Kd_{bs}, because the value varies, depending on the fraction of organic carbon in bottom sediment. Recommended Kd_{bs} value was calculated by using the K_{oc} value that is provided in this table.	1.24E+01
ksg (year)$^{-1}$	*Ksg* value was calculated by using the chemical half-life in soil, as cited in Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	9.03E+00
Fv (unitless)	*Fv* value was calculated by using equations cited in Junge (1977) and Bidleman (1988). Recommended value of *Fv* was calculated by using T_m and *Vp* values that are provided in this table.	1.00

Note:
NA = Not applicable
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

TABLE A-2-204

CHEMICAL-SPECIFIC INPUTS FOR ZINC (7440-66-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	65.38
T_m (^{o}K)	Budavari, O'Neil, Smith, and Heckelman (1989)	692.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water. OR Budavari, O'Neil, Smith, and Heckelman (1989)	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.17E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.36E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996b), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	6.2E+01 at pH=6.8
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	6.2E+01 at pH=6.8
Kd_{bs} (mL/g)	Kd_{bs} value is assumed to be same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in U.S. EPA (1994f).	6.2E+01 at pH=6.8
ksg (year)$^{-1}$	--	ND
Fv (unitless)	Because they are nonvolatile, metals are assumed to be 100 percent in particulate phase and zero percent in the vapor phase, as cited in U.S. EPA (1994f).	0.0

Note:
NA = Not applicable;
ND = No data available

All parameters are defined in LIST OF VARIABLES on page A-2-ii.

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Screening Level Ecological Risk Assessment Protocol for Hazardous Waste Combustion Facilities

Volume Three
Appendices B to H

Peer Review Draft

APPENDIX B

ESTIMATING MEDIA CONCENTRATION EQUATIONS AND VARIABLE VALUES

Screening Level Ecological Risk Assessment Protocol

August 1999

APPENDIX B

TABLE OF CONTENTS

TABLE **PAGE**

APPENDIX B

TABLE OF CONTENTS

APPENDIX B

LIST OF VARIABLES AND PARAMETERS

γ	=	Empirical constant (unitless)
λ_z	=	Dimensionless viscous sublayer thickness (unitless)
μ_a	=	Viscosity of air (g/cm-s)
μ_w	=	Viscosity of water corresponding to water temperature (g/cm-s)
ρ_a	=	Density of air (g/cm^3 or g/m^3)
ρ_w	=	Density of water corresponding to water temperature (g/cm^3)
θ	=	Temperature correction factor (unitless)
θ_{bs}	=	Bed sediment porosity (L volume/L sediment)—unitless
θ_{sw}	=	Soil volumetric water content (mL water/cm^3 soil)
a	=	Empirical intercept coefficient (unitless)
A	=	Surface area of contaminated area (m^2)
A_I	=	Impervious watershed area receiving COPC deposition (m^2)
A_L	=	Total watershed area receiving COPC deposition (m^2)
A_W	=	Water body surface area (m^2)
b	=	Empirical slope coefficient (unitless)
BD	=	Soil bulk density (g soil/cm^3 soil)
$BCFr$	=	Plant-soil biotransfer factor (mg COPC/kg DW plant)/(mg COPC/kg soil)—unitless
BS	=	Benthic solids concentration (g sediment/cm^3 sediment)
Bs	=	Soil bioavailability factor (unitless)
Bv	=	Air-to-plant biotransfer factor (mg COPC/kg DW plant)/(mg COPC/kg air)—unitless
c	=	Junge constant = 1.7×10^{-4} (atm-cm)
C	=	USLE cover management factor (unitless)
C_d	=	Drag coefficient (unitless)
C_{dw}	=	Dissolved phase water concentration (mg COPC/L water)
C_{hp}	=	Unitized hourly air concentration from vapor phase (µg-s/g-m^3)
C_{hv}	=	Unitized hourly air concentration from particle phase (µg-s/g-m^3)
Cs	=	COPC concentration in soil (mg COPC/kg soil)
C_{sed}	=	COPC concentration in bed sediment (mg COPC/kg sediment)
C_{wctot}	=	Total COPC concentration in water column (mg COPC/L water column)
C_{wtot}	=	Total water body COPC concentration including water column and bed sediment (g COPC/m^3 water body) or (mg/L)
Cyp	=	Unitized yearly average air concentration from particle phase (µg-s/g-m^3)
Cyv	=	Unitized yearly average air concentration from vapor phase (µg-s/g-m^3)
$Cywv$	=	Unitized yearly average air concentration from vapor phase (over water body or watershed) (µg-s/g-m^3)
D_a	=	Diffusivity of COPC in air (cm^2/s)
d_{bs}	=	Depth of upper benthic sediment layer (m)

Ds	=	Deposition term (mg COPC/kg soil-yr)
d_{wc}	=	Depth of water column (m)
D_w	=	Diffusivity of COPC in water (cm^2/s)
$Dydp$	=	Unitized yearly average dry deposition from particle phase (s/m^2-yr)
$Dytwp$	=	Unitized yearly average total (wet and dry) deposition from particle phase (over water body or watershed) (s/m^2-yr)
$Dywp$	=	Unitized yearly average wet deposition from particle phase (s/m^2-yr)
$Dywv$	=	Unitized yearly average wet deposition from vapor phase (s/m^2-yr)
$Dywwv$	=	Unitized yearly average wet deposition from vapor phase (over water body or watershed) (s/m^2-yr)
d_z	=	Total water body depth (m)
ER	=	Soil enrichment ratio (unitless)
E_v	=	Average annual evapotranspiration (cm/yr)
f_{bs}	=	Fraction of total water body COPC concentration in benthic sediment (unitless)
Fd	=	Fraction of diet that is soil (unitless)
Fw	=	Fraction of COPC wet deposition that adheres to plant surfaces (unitless)
f_{wc}	=	Fraction of total water body COPC concentration in the water column (unitless)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
H	=	Henry's Law constant (atm-m^3/mol)
I	=	Average annual irrigation (cm/yr)
k	=	Von Karman's constant (unitless)
K	=	USLE erodibility factor (ton/acre)
k_b	=	Benthic burial rate constant (yr^{-1})
Kd_{bs}	=	Bed sediment/sediment pore water partition coefficient (cm^3 water/g bottom sediment or L water/kg bottom sediment)
Kd_s	=	Soil-water partition coefficient (cm^3 water/g soil)
Kd_{sw}	=	Suspended sediment-surface water partition coefficient (L water/kg suspended sediment)
K_G	=	Gas phase transfer coefficient (m/yr)
K_L	=	Liquid phase transfer coefficient (m/yr)
K_{oc}	=	Soil organic carbon-water partition coefficient (mL water/g soil)
K_{ow}	=	Octanol-water partition coefficient (mg COPC/L octanol)/(mg COPC/L octanol)—unitless
kp	=	Plant surface loss coefficient (yr^{-1})
ks	=	COPC soil loss constant due to all processes (yr^{-1})
kse	=	COPC loss constant due to soil erosion (yr^{-1})
ksg	=	COPC loss constant due to biotic and abiotic degradation (yr^{-1})
ksl	=	COPC loss constant due to leaching (yr^{-1})
ksr	=	COPC loss constant due to surface runoff (yr^{-1})
ksv	=	COPC loss constant due to volatilization (yr^{-1})
k_v	=	Water column volatilization rate constant (yr^{-1})
K_v	=	Overall COPC transfer rate coefficient (m/yr)
k_{wt}	=	Overall total water body dissipation rate constant (yr^{-1})

L_{DEP}	=	Total (wet and dry) particle phase and wet vapor phase COPC direct deposition load to water body (g/yr)
L_{Dif}	=	Vapor phase COPC diffusion (dry deposition) load to water body (g/yr)
L_E	=	Soil erosion load (g/yr)
L_R	=	Runoff load from pervious surfaces (g/yr)
L_{RI}	=	Runoff load from impervious surfaces (g/yr)
L_T	=	Total COPC load to the water body (including deposition, runoff, and erosion) (g/yr)
LS	=	USLE length-slope factor (unitless)
OC_{sed}	=	Fraction of organic carbon in bottom sediment (unitless)
p°_L	=	Liquid phase vapor pressure of chemical (atm)
p°_S	=	Solid phase vapor pressure of chemical (atm)
P	=	Average annual precipitation (cm/yr)
PF	=	USLE supporting practice factor (unitless)
Pd	=	Plant concentration due to direct deposition (mg COPC/kg DW)
Pr	=	Plant concentration due to root uptake (mg COPC/kg DW)
Pv	=	Plant concentration due to air-to-plant transfer (µg COPC/g DW plant tissue or mg COPC/kg DW plant tissue)
Q	=	COPC-specific emission rate (g/s)
r	=	Interception fraction—the fraction of material in rain intercepted by vegetation and initially retained (unitless)
R	=	Universal gas constant (atm-m^3/mol-K)
RO	=	Average annual surface runoff from pervious areas (cm/yr)
RF	=	USLE rainfall (or erosivity) factor (yr^{-1})
Rp	=	Interception fraction of the edible portion of plant (unitless)
SD	=	Sediment delivery ratio (unitless)
ΔSf	=	Entropy of fusion [$\Delta S_f/R$ = 6.79 (unitless)]
SF	=	Slope factor $(mg/kg\text{-}day)^{-1}$
S_T	=	Whitby's average surface area of particulates (aerosols) = 3.5×10^{-6} cm^2/cm^3 air for background plus local sources = 1.1×10^{-5} cm^2/cm^3 air for urban sources
T_a	=	Ambient air temperature (K)
T_1	=	Time period at the beginning of combustion (yr)
T_2	=	Length of exposure duration (yr)
tD	=	Time period over which deposition occurs (or time period of combustion) (yr)
T_m	=	Melting point of chemical (K)
Tp	=	Length of plant exposure to deposition per harvest of edible portion of plant (yr)
TSS	=	Total suspended solids concentration (mg/L)
T_{wk}	=	Water body temperature (K)
$t_{1/2}$	=	Half-time of COPC (days)

u	=	Current velocity (m/s)
Vdv	=	Dry deposition velocity (cm/s)
Vf_x	=	Average volumetric flow rate through water body (m^3/yr)
W	=	Average annual wind speed (m/s)
X_e	=	Unit soil loss (kg/m^2-yr)
Yh	=	Dry harvest yield = 1.22×10^{11} kg DW, calculated from the 1993 U.S. average wet weight Yh of 1.35×10^{11} kg (USDA 1994b) and a conversion factor of 0.9 (Fries 1994)
Yh_i	=	Harvest yield of *i*th crop (kg DW)
Yp	=	Yield or standing crop biomass of the edible portion of the plant (productivity) (kg DW/m^2)
Z_s	=	Soil mixing zone depth (cm)
0.01	=	Units conversion factor (kg cm^2/mg-m^2)
10^{-6}	=	Units conversion factor (g/µg)
10^{-6}	=	Units conversion factor (kg/mg)
0.31536	=	Units conversion factor (m-g-s/cm-µg-yr)
365	=	Units conversion factor (days/yr)
907.18	=	Units conversion factor (kg/ton)
0.1	=	Units conversion factor (g-kg/cm^2-m^2)
0.001	=	Units conversion factor (kg-cm^2/mg-m^2)
100	=	Units conversion factor (mg-cm^2/kg-cm^2)
1000	=	Units conversion factor (mg/g)
4047	=	Units conversion factor (m^2/acre)
1×10^3	=	Units conversion factor (g/kg)
3.1536×10^7	=	Units conversion factor (s/yr)

TABLE B-1-1

SOIL CONCENTRATION DUE TO DEPOSITION
(SOIL EQUATIONS)

Description

The equation in this table is used to calculate the highest annual average COPC concentration in soil resulting from wet and dry deposition of particles and vapors to soil. COPCs are assumed to be incorporated only to a finite depth (the soil mixing depth, Z_s).

The highest annual average COPC concentration in soil is assumed to occur at the end of the time period of combustion. The following uncertainty is associated with this variable:

(1) The time period for deposition of COPCs resulting from hazardous waste combustion is assumed to be a conservative, long-term value.
(2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with in-situ materials), in comparison to that of other residues. This uncertainty may underestimate *Cs*.

TABLE B-1-1

SOIL CONCENTRATION DUE TO DEPOSITION
(SOIL EQUATIONS)

(Page 2 of 9)

Equation

Highest Annual Average Soil Concentration

$$Cs = \frac{Ds \cdot [1 - \exp(-ks \cdot tD)]}{ks}$$

where:

$$Ds = \frac{100 \cdot Q}{Z_s \cdot BD} \cdot [F_v\ (0.31536 \cdot Vdv \cdot Cyv + Dywv) + (Dydp + Dywp) \cdot (1 - F_v)]$$

For mercury modeling:

$$Ds_{Mercury} = \frac{100 \cdot (0.48 Q_{TotalMercury})}{Z_s \cdot BD} \cdot [F_{v_{Hg^{2+}}}\ (0.31536 \cdot Vdv \cdot Cyv + Dywv) + (Dydp + Dywp) \cdot (1 - F_{v_{Hg^{2+}}})]$$

In calculating *Cs* for mercury comounds, *Ds(Mercury)* is calculated as shown above using the total mercury emission rate (*Q*) measured at the stack and F_v for mercuric chloride (F_v = 0.85). As presented below, the calculated *Ds(Mercury)* value is apportioned into the divalent mercury (Hg^{2+}) and methyl mercury (MHg) forms based on a 98% Hg^{2+} and 2% MHg speciation split in dry land soils, and a 85% Hg^{2+} and 15% MHg speciation split in wetland soils (see Chapter 2).

For Calculating *Cs* in Dry Land Soils		**For Calculating *Cs* in Wetland Soils**	
Ds (Hg^{2+}) =	0.98 *Ds(Mercury)*	*Ds* (Hg^{2+}) =	0.85 *Ds(Mercury)*
Ds (MHg) =	0.02 *Ds(Mercury)*	*Ds* (MHg) =	0.15 *Ds(Mercury)*
Ds (Hg^0) =	0.0	*Ds* (Hg^0) =	0.0

Calculate *Cs* for divalent and methyl mercury using the corresponding (1) fate and transport parameters for mercuric chloride (divalent mercury) and methyl mercury (provided in Appendix A-2), and (2) *Ds* (Hg^{2+}) and *Ds* (MHg) as calculated above. After calculating species specific *Cs* values, divalent and methyl mercury should continue to be modeled throughout Appendix B equations as individual COPCs.

Variable	Description	Units	Value
Cs	COPC concentration in soil	mg COPC/kg soil	

TABLE B-1-1

SOIL CONCENTRATION DUE TO DEPOSITION
(SOIL EQUATIONS)

(Page 3 of 9)

Variable	Description	Units	Value
Ds	Deposition term	mg COPC/kg soil/yr	**Varies (calculated - Table B-1-1)** Consistent with U.S. EPA (1994a; 1998), U.S. EPA OSW recommends incorporating the use of a deposition term into the *Cs* equation. Uncertainties associated with this variable include the following: (1) Five of the variables in the equation for *Ds (Q, Cyv, Dywv, Dywp* and *Dydp*) are COPC- and site-specific measured or modeled variables. The direction and magnitude of any uncertainties should not be generalized. Uncertainties associated with these variables will probably be different at each facility. (2) Based on the narrow recommended ranges, uncertainties associated with *Vdv*, F_v, and *BD* are expected to be small. (3) Values for Z_s vary by about one order of magnitude. Uncertainty is greatly reduced if it is known whether soils are tilled or untilled.
tD	Time period over which deposition occurs (time period of combustion)	yr	**100** U.S. EPA (1990a) specified that this period of time can be represented by 30, 60 , or 100 years. U.S. EPA OSW recommends that facilities use the conservative value of 100 years unless site-specific information is available indicating that this assumption is unreasonable.
ks	COPC soil loss constant due to all processes	yr^{-1}	**Varies (calculated - Table B-1-2)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-1-2. Soil loss constant is the sum of all COPC removal processes. Uncertainties associated with this variable are discussed in Table B-1-2.
100	Units conversion factor	m^2-mg/cm^2-kg	

TABLE B-1-1

SOIL CONCENTRATION DUE TO DEPOSITION
(SOIL EQUATIONS)

(Page 4 of 9)

Variable	Description	Units	Value
Q	COPC-specific emission rate	g/s	**Varies (site-specific)** This variable is COPC- and site-specific (see Chapters 2 and 3). Uncertainties associated with this variable are site-specific.
Z_s	Soil mixing zone depth	cm	**1 or 20** Z_s should be computed for two depth intervals. U.S. EPA OSW recommends the following values for this variable: Soil — Depth (cm) Untilled — 1 Tilled — 20 The following uncertainty is associated with this variable: (1) For soluble COPCs, leaching might lead to movement to below soil depths and justify a greater mixing depth. This uncertainty may overestimate *Cs*. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution, in comparison to that of other residues. This uncertainty may underestimate *Cs*.
BD	Soil bulk density	g/cm^3	**1.5** This variable is affected by the soil structure, such as looseness or compaction of the soil, depending on the water and clay content of the soil (Hillel 1980), as summarized in U.S. EPA (1990a). A proposed range of 0.83 to 1.84 was originally cited in Hoffman and Baes (1979). U.S. EPA (1994c) recommends a default *BD* value of 1.5 g/cm^3, based on a mean value for loam soil that was obtained from Carsel, Parrish, Jones, Hansen, and Lamb (1988). The value of 1.5 g/cm^3 also represents the midpoint of the "relatively narrow range" for *BD* of 1.2 to 1.7 g/cm^3 (U.S. EPA 1993a). The following uncertainty is associated with this variable: (1) The recommended range of *BD* values may not accurately represent site-specific soil conditions.

TABLE B-1-1

SOIL CONCENTRATION DUE TO DEPOSITION
(SOIL EQUATIONS)

(Page 5 of 9)

Variable	Description	Units	Value
F_v	Fraction of COPC air concentration in vapor phase	unitless	**0 to 1 (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-2. Values are also presented in U.S. EPA (1993), RTI (1992), and NC DEHNR (1997) based on the work of Bidleman (1988), as cited in U.S. EPA (1994c). The following uncertainty is associated with this variable: (1) It is based on the assumption of a default S_T value for background plus local sources, rather than an S_T value for urban sources. If a specific site is located in an urban area, the use of the latter S_T value may be more appropriate. Specifically, the S_T value for urban sources is about one order of magnitude greater than that for background plus local sources, and it would result in a lower calculated F_v value; however, the F_v value is likely to be only a few percent lower. (2) According to Bidleman (1988), the equation used to calculate F_v assumes that the variable c (Junge constant) is constant for all chemicals. However, the value of c depends on the chemical (sorbate) molecular weight, the surface concentration for monolayer coverage, and the difference between the heat of desorption from the particle surface and the heat of vaporization of the liquid-phase sorbate. To the extent that site- or COPC-specific conditions may cause the value of c to vary, uncertainty is introduced if a constant value of c is used to calculate F_v.
0.31536	Units conversion factor	m-g-s/cm-µg-yr	
Vdv	Dry deposition velocity	cm/s	**3** U.S. EPA (1994c) recommended the use of 3 cm/s for the dry deposition velocity, based on median dry deposition velocity for HNO_3 from an unspecified U.S. EPA database of dry deposition velocities for HNO_3, ozone, and SO_2. HNO_3 was considered the most similar to the COPCs recommended for consideration. The value should be applicable to any organic COPC with a low Henry's Law Constant. The following uncertainty is associated with this variable: (1) HNO_3 may not adequately represent specific COPCs with high Henry's Law Constant values. Therefore, the use of a single value may under- or overestimate estimated soil concentration.

TABLE B-1-1

SOIL CONCENTRATION DUE TO DEPOSITION
(SOIL EQUATIONS)

(Page 6 of 9)

Variable	Description	Units	Value
Cyv	Unitized yearly average air concentration from vapor phase	µg-s/g-m^3	**Varies (modeled)** This variable is COPC- and site-specific, and is determined by air dispersion modeling (see Chapter 3). Uncertainties associated with this variable are site-specific.
Dywv	Unitized yearly average wet deposition from vapor phase	s/m^2-yr	**Varies (modeled)** This variable is COPC- and site-specific, and is determined by air dispersion modeling (see Chapter 3). Uncertainties associated with this variable are site-specific.
Dydp	Unitized yearly average dry deposition from particle phase	s/m^2-yr	**Varies (modeled)** This variable is COPC- and site-specific, and is determined by air dispersion modeling (see Chapter 3). Uncertainties associated with this variable are site-specific.
Dywp	Unitized yearly average wet deposition from particle phase	s/m^2-yr	**Varies (modeled)** This variable is COPC- and site-specific, and is determined by air dispersion modeling (see Chapter 3). Uncertainties associated with this variable are site-specific.

TABLE B-1-1

SOIL CONCENTRATION DUE TO DEPOSITION (SOIL EQUATIONS)

(Page 7 of 9)

REFERENCES AND DISCUSSION

Bidleman, T.F. 1988. "Atmospheric Processes." *Environmental Science and Technology*. Volume 22. Number 4. Pages 361-367.

This reference is for the statement that the equation used to calculate the fraction of air concentration in vapor phase (F_v) assumes that the variable c (the Junge constant) is constant for all chemicals. However, this document notes that the value of c depends on the chemical (sorbate) molecular weight, the surface concentration for monolayer coverage, and the difference between the heat of desorption from the particle surface and the heat of vaporization of the liquid-phase sorbate. The following equation, presented in this document, is cited by U.S. EPA (1994c) and NC DEHNR (1997) for calculating the variable F_v:

$$F_v = 1 - \frac{c \cdot S_T}{P^\circ_L + c \cdot S_T}$$

where:

F_v	=	Fraction of chemical air concentration in vapor phase (unitless)
c	=	Junge constant = 1.7 E-04 (atm-cm)
S_T	=	Whitby's average surface area of particulates = 3.5 E-06 cm^2/cm^3 air (corresponds to background plus local sources)
P°_L	=	Liquid-phase vapor pressure of chemical (atm) (see Appendix A-2)

If the chemical is a solid at ambient temperatures, the solid-phase vapor pressure is converted to a liquid-phase vapor pressure as follows:

$$\ln \frac{P^\circ_L}{P^\circ_S} = \frac{\Delta S_f}{R} \cdot \frac{(T_m - T_a)}{T_a}$$

where:

P°_S	=	Solid-phase vapor pressure of chemical (atm) (see Appendix A-2)
$\frac{\Delta S_f}{R}$	=	Entropy of fusion over the universal gas constant = 6.79 (unitless)
T_m	=	Melting point of chemical (K) (see Appendix C)
T_a	=	Ambient air temperature = 298 K (25°C)

Carsel, R.F., R.S. Parrish, R.L. Jones, J.L. Hansen, and R.L. Lamb. 1988. "Characterizing the Uncertainty of Pesticide Leaching in Agricultural Soils." *Journal of Contaminant Hydrology*. Vol. 2. Pages 11-24.

This reference is cited by U.S. EPA (1994b) as the source for a mean soil bulk density value of 1.5 g/cm^3 for loam soil.

Hillel, D. 1980. *Fundamentals of Soil Physics*. Academic Press, Inc. New York.

This document is cited by U.S. EPA (1990a) for the statement that dry soil bulk density, *BD*, is affected by the soil structure, such as looseness or compaction of the soil, depending on the water and clay content of the soil.

Hoffman, F.O., and C.F. Baes, 1979. *A Statistical Analysis of Selected Parameters for Predicting Food Chain Transport and Internal Dose of Radionuclides*. ORNL/NOREG/TM-882.

This document presents a soil bulk density range, *BD*, of 0.83 to 1.84.

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units*. January.

This is one of the source documents for for the equation in Table B-1-1. This document also recommends the use of (1) a deposition term, *Ds*, and (2) COPC-specific F_v (fraction of COPC air concentration in vapor phase) values.

Research Triangle Institute (RTI). 1992. *Preliminary Soil Action Level for Superfund Sites.* Draft Interim Report. Prepared for U.S. EPA Hazardous Site Control Division, Remedial Operations Guidance Branch. Arlington, Virginia. EPA Contract 68-W1-0021. Work Assignment No. B-03, Work Assignment Manager Loren Henning. December.

This document is a reference source for COPC-specific F_v (fraction of COPC air concentration in vapor phase) values.

U.S. EPA. 1990a. *Interim Final Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Environmental Criteria and Assessment Office. Office of Research and Development. EPA 600-90-003. January.

This document is a reference source for the equation in Table B-1-1, and it recommends that (1) the time period over which deposition occurs (time period for combustion), *tD*, be represented by periods of 30, 60, and 100 years, and (2) undocumented values for soil mixing zone depth, Z_s, for tilled and untilled soil.

U.S. EPA. 1993. *Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. Working Group Recommendations. Office of Solid Waste. Office of Research and Development. Washington, D.C. September 24.

This document is a reference for the equation in Table B-1-1. It recommends using a deposition term, *Ds*, and COPC-specific F_v values (fraction of COPC air concentration in vapor phase) in the *Cs* equation.

U.S. EPA 1994a. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities.* Office of Emergency and Remedial Response. Office of Solid Waste. April 15.

TABLE B-1-1

SOIL CONCENTRATION DUE TO DEPOSITION
(SOIL EQUATIONS)

(Page 9 of 9)

This document is a reference for the equation in Table B-1-1; it recommends that the following be used in the *Cs* equation: (1) a deposition term, *Ds*, and (2) a default soil dry bulk density value of 1.5 g/cm^3, based on a mean value for loam soil from Carsel, Parrish, Jones, Hansen, and Lamb (1988).

U.S. EPA. 1994b. *Estimating Exposure to Dioxin-Like Compounds. Volume III: Site-Specific Assessment Procedures.* Review Draft. Office of Research and Development. Washington, D.C. June. EPA/600/6-88/005Cc.

U.S. EPA. 1994c. *Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes*. Office of Emergency and Remedial Response. Office of Solid Waste. December 14.

The value for dry deposition velocity is based on median dry deposition velocity for HNO_3 from a U.S. EPA database of dry deposition velocities for HNO3 ozone, and SO_2. HNO_3 was considered the most similar to the constituents covered and the value should be applicable to any organic compound having a low Henry's Law Constant. The reference document for this recommendation was not cited. This document recommends the following:

- F_v values (fraction of COPC air concentration in vapor phase) that range from 0.27 to 1 for organic COPCs
- *Vdv* value (dry deposition velocity) of 3 cm/s (however, no reference is provided for this recommendation)
- Default soil dry bulk density value of 1.5 g/cm^3, based on a mean for loam soil from Carsel, Parrish, Jones, Hansen, and Lamb (1988)
- *Vdv* value of 3 cm/s, based on median dry deposition velocity for HNO_3 from an unspecified U.S. EPA database of dry deposition velocities for HNO_3, ozone, and SO_2. HNO_3 was considered the most similar to the COPCs recommended for consideration.

U.S. EPA. 1998. "Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilitites." External Peer Review Draft. U.S. EPA Region 6 and U.S. EPA OSW. Volumes 1-3. EPA530-D-98-001A. July.

TABLE B-1-2

COPC SOIL LOSS CONSTANT DUE TO ALL PROCESSES
(SOIL EQUATIONS)

Description

This equation calculates the soil loss constant (*ks*), which accounts for the loss of COPCs from soil by several mechanisms.

Uncertainties associated with this equation include the following:

(1) COPC-specific values for *ksg* are empirically determined from field studies. No information is available regarding the application of these values to the site-specific conditions associated with affected facilities.

Equation

$$ks = ksg + kse + ksr + ksl + ksv$$

Variable	Description	Units	Value
ks	COPC soil loss constant due to all processes	yr^{-1}	
ksg	COPC loss constant due to biotic and abiotic degradation	yr^{-1}	**Varies (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-2. "Degradation rate" values are also presented in NC DEHNR (1997). However, no reference or source is provided for the values. U.S. EPA (1994a and 1994b) state that *ksg* values are COPC-specific; however, all *ksg* values are presented as zero (U.S. EPA 1994a) or as "NA" (U.S. EPA 1994b). The basis of these assumptions is not addressed. The following uncertainty is associated with this variable: (1) COPC-specific values for *ksg* are empirically determined from field studies. No information is available regarding the application of these values to the site-specific conditions associated with affected facilities.

TABLE B-1-2

COPC SOIL LOSS CONSTANT DUE TO ALL PROCESSES
(SOIL EQUATIONS)

Variable	Description	Units	Value
kse	COPC loss constant due to soil erosion	yr^{-1}	**0** This variable is COPC- and site-specific, and is further discussed in Table B-1-3. Consistent with U.S. EPA (1994a; 1994b; 1998) and NC DEHNR (1997), U.S. EPA OSW recommends that the default value assumed for *kse* is zero because of contaminated soil eroding onto the site and away from the site. Uncertainties associated with this variable include the following: (1) The source of the equation in Table B-1-3 has not been identified. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with in-situ materials), in comparison to that of other residues. This uncertainty may underestimate *kse*.
ksr	COPC loss constant due to surface runoff	yr^{-1}	**Varies (calculated - Table B-1-4)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-1-4. No reference document is cited for this equation. The use of this equation is consistent with U.S. EPA (1994b; 1998) and NC DEHNR (1997). U.S. EPA (1994a) states that all *ksr* values are zero but does not explain the basis of this assumption. Uncertainties associated with this variable include the following: (1) The source of the equation in Table B-1-4 has not been identified. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with in-situ materials), in comparison to that of other residues. This uncertainty may underestimate *ksr*.
ksl	COPC loss constant due to leaching	yr^{-1}	**Varies (calculated - Table B-1-5)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-1-5. No reference document is cited for this equation. The use of this equation is consistent with U.S. EPA (1993; 1994b; 1998), and NC DEHNR (1997). U.S. EPA (1994a) states that all *ksl* values are zero but does not explain the basis of this assumption. Uncertainties associated with this variable include the following: (1) The source of the equation in Table B-1-5 has not been identified. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with in-situ materials), in comparison to that of other residues. This uncertainty may underestimate *ksl*.

TABLE B-1-2

COPC SOIL LOSS CONSTANT DUE TO ALL PROCESSES
(SOIL EQUATIONS)

Variable	Description	Units	Value
ksv	COPC loss constant due to volatilization	yr^{-1}	**Varies (calculated - Table B-1-6)** This variable is COPC- and site-specific, and is calculated using the equation in Table B-1-6. Uncertainties associated with this variable include the following: (1) Deposition to hard surfaces may result in dust residues that have negligible dilution, (as a result of potential mixing with in-situ materials), in comparison to that of other residues. This uncertainty may underestimate *ksv*.

TABLE B-1-2

COPC SOIL LOSS CONSTANT DUE TO ALL PROCESSES (SOIL EQUATIONS)

REFERENCES AND DISCUSSION

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units.* January.

This document is one of the reference documents for the equations in Tables B-1-4, B-1-5, and B-1-6. No source for these equations has been identified. This document is also cited as (1) the source for a range of COPC-specific degradation rates (*ksg*), and (2) one of the sources that recommend using the assumption that the loss resulting from erosion (*kse*) is zero because of contaminated soil eroding onto the site and away from the site.

U.S. EPA. 1993. *Review Draft Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Office of Health and Environmental Assessment. Office of Research and Development. EPA-600-AP-93-003. November 10.

This document is one of the reference documents for the equations in Tables B-1-4 and B-1-5.

U.S. EPA. 1994a. *Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities.* April 15.

This document is cited as a source for the assumptions regarding losses resulting from erosion (*kse*), surface runoff (*ksr*), degradation (*ksg*), and leaching (*ksl*), and volatilization (*ksv*).

U.S. EPA. 1994b. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities.* Office of Emergency and Remedial Response. Office of Solid Waste. December 14.

This document is one of the reference documents for the equations in Tables B-1-4 and B-1-5. This document is also cited as one of the sources that recommend using the assumption that the loss resulting from erosion (*kse*) is zero and the loss resulting from degradation (*ksg*) is "NA" or zero for all compounds.

U.S. EPA. 1998. "Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilitites." External Peer Review Draft. U.S. EPA Region 6 and U.S. EPA OSW. Volumes 1-3. EPA530-D-98-001A. July.

TABLE B-1-3

COPC LOSS CONSTANT DUE TO SOIL EROSION (SOIL EQUATIONS)

Description

This equation calculates the constant for COPC loss resulting from erosion of soil. Consistent with U.S. EPA (1994), U.S. EPA (1994b), NC DEHNR (1997), and U.S. EPA (1998), U.S. EPA OSW recommends that the default value assumed for *kse* is zero because of contaminated soil eroding onto the site and away from the site. In site-specific cases where the permitting authority considers it appropriate to calculate a *kse*, the following equation presented in this table should be considered along with associated uncertainties. Additional discussion on the determination of *kse* can be obtained from review of the methodologies described in U.S. EPA NCEA document, *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (In Press).

Uncertainties associated with this equation include:

(1) For soluble COPCs, leaching might lead to movement below 1 cm in soils and justify a greater mixing depth. This uncertainty may overestimate *kse*.
(2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with in-situ materials) in comparison to that of other residues. This uncertainty may underestimate *kse*.

Equation

$$kse = \frac{0.1 \cdot X_e \cdot SD \cdot ER}{BD \cdot Z_s} \cdot \left(\frac{Kd_s \cdot BD}{\theta_{sw} + (Kd_s \cdot BD)} \right)$$

Variable	Description	Units	Value
kse	COPC loss constant due to soil erosion	yr^{-1}	**0** Consistent with U.S. EPA (1994), U.S. EPA (1994b), U.S. EPA (1998), and NC DEHNR (1997), U.S. EPA OSW recommends that the default value assumed for *kse* is zero because of contaminated soil eroding onto the site and away from the site.
0.1	Units conversion factor	$g\text{-}kg/cm^2\text{-}m^2$	

TABLE B-1-3

COPC LOSS CONSTANT DUE TO SOIL EROSION
(SOIL EQUATIONS)

(Page 2 of 6)

Variable	Description	Units	Value
X_e	Unit soil loss	kg/m^2-yr	**Varies (calculated - Table B-2-7)** This variable is site-specific and is calculated by using the equation in Table B-2-7. The following uncertainty is associated with this variable: (1) All of the equation variables are site-specific. Use of default values rather than site-specific values for any or all of these variables will result in unit soil loss (X_e) estimates that are under- or overestimated to some degree. Based on default values, X_e estimates can vary over a range of less than two orders of magnitude.
SD	Sediment delivery ratio	unitless	**Varies (calculated - Table B-2-8)** This value is site-specific and is calculated by using the equation in Table B-2-8. Uncertainties associated with this variable include the following: (1) The recommended default values for the empirical intercept coefficient, *a*, are average values that are based on studies of sediment yields from various watersheds. Therefore, those default values may not accurately represent site-specific watershed conditions. As a result, use of these default values may under- or overestimate *SD*. (2) The recommended default value for the empirical slope coefficient, *b*, is based on a review of sediment yields from various watersheds. This single default value may not accurately represent site-specific watershed conditions. As a result, use of this default value may under- or overestimate *SD*.
ER	Soil enrichment ratio	unitless	**Inorganics: 1** **Organics: 3** COPC enrichment occurs because (1) lighter soil particles erode more than heavier soil particles, and (2) concentration of organic COPCs—which is a function of organic carbon content of sorbing media—is expected to be higher in eroded material than in in-situ soil (U.S. EPA 1993). In the absence of site-specific data, U.S. EPA OSW recommends a default value of 3 for organic COPCs and 1 for inorganic COPCs. This is consistent with other U.S. EPA guidance (1993), which recommends a range of 1 to 5 and a value of 3 as a "reasonable first estimate." This range has been used for organic matter, phosphorus, and other soil-bound COPCs (U.S. EPA 1993); however, no sources or references were provided for this range. *ER* is generally higher in sandy soils than in silty or loamy soils (U.S. EPA 1993). The following uncertainty is associated with this variable: (1) The default ER value may not accurately reflect site-specific conditions; therefore, *kse* may be over- or underestimated to an unknown extent.

TABLE B-1-3

COPC LOSS CONSTANT DUE TO SOIL EROSION
(SOIL EQUATIONS)

Variable	Description	Units	Value
BD	Soil bulk density	g/cm^3	**1.5** This variable is affected by the soil structure, such as looseness or compaction of the soil, depending on the water and clay content of the soil (Hillel 1980), as summarized in U.S. EPA (1990). A range of 0.83 to 1.84 was originally cited in Hoffman and Baes (1979). U.S. EPA (1994) recommends a default BD value of 1.5 g/cm^3, based on a mean value for loam soil that was taken from Carsel, Parrish, Jones, Hansen, and Lamb (1988). The value of 1.5 g/cm^3 also represents the midpoint of the "relatively narrow range" for *BD* of 1.2 to 1.7 g/cm^3 (U.S. EPA 1993). The following uncertainty is associated with this variable: (1) The recommended range of soil dry bulk density values may not accurately represent site-specific soil conditions.
Z_s	Soil mixing zone depth	cm	**1 or 20** U.S. EPA OSW recommends the following values for this variable: Soil — Depth (cm) Untilled — 1 Tilled — 20 The following uncertainty is associated with this variable: (1) For soluble COPCs, leaching might lead to movement to below 1 cm in soils and justify a greater mixing depth. This uncertainty may overestimate *kse*. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with in-situ materials), in comparison to that of other residues. This uncertainty may underestimate *kse*.
Kd_s	Soil-water partition coefficient	cm^3/g	**Varies (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-2. The following uncertainty is associated with this variable: (1) Uncertainties associated with this parameter will be limited if Kd_s values are determined as described in Appendix A-2.

TABLE B-1-3

COPC LOSS CONSTANT DUE TO SOIL EROSION
(SOIL EQUATIONS)

Variable	Description	Units	Value
θ_{sw}	Soil volumetric water content	mL/cm^3	**0.2** This variable depends on the available water and on soil structure. θ_{sw} can be estimated as the midpoint between a soil's field capacity and wilting point, if a representative watershed soil can be identified. However, U.S. EPA OSW recommends the use of 0.2 mL/cm^3 as a default value. This value is the midpoint of the range 0.1 (very sandy soils) to 0.3 (heavy loam/clay soils) recommended by U.S. EPA (1993) (no source or reference is provided for this range) and is consistent with U.S. EPA (1994). The following uncertainty is associated with this variable: (1) The default θ_{sw} values may not accurately reflect site-specific or local conditions; therefore, *kse* may be under- or overestimated to a small extent, based on the limited range of values.

TABLE B-1-3

COPC LOSS CONSTANT DUE TO SOIL EROSION (SOIL EQUATIONS)

REFERENCES AND DISCUSSION

Carsel, R.F., R.S. Parish, R.L. Jones, J.L. Hansen, and R.L. Lamb. 1988. "Characterizing the Uncertainty of Pesticide Leaching in Agricultural Soils." *Journal of Contaminant Hydrology*. Vol. 2. Pages 11-24.

This document is cited by U.S. EPA (1994) as the source for a mean soil bulk density, *BD*, value of 1.5 g/cm^3 for loam soil.

Hillel, D. 1980. *Fundamentals of Soil Physics.* Academic Press, Inc. New York.

This document is cited by U.S. EPA (1990) for the statement that dry soil bulk density, *BD*, is affected by the soil structure, such as looseness or compaction of the soil, depending on the water and clay content of the soil.

Hoffman, F.O., and C.F. Baes. 1979. *A Statistical Analysis of Selected Parameters for Predicting Food Chain Transport and Internal Dose of Radionuclides*. ORNL/NUREG/TM-882.

This document presents a soil bulk density, *BD*, range of 0.83 to 1.84.

NC DEHNR. 1997. *Draft NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units*. January.

U.S. EPA. 1990. *Interim Final Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Environmental Criteria and Assessment Office. Office of Research and Development. EPA 600-90-003. January.

This document presents a range of values for soil mixing zone depth, Z_s, for tilled and untilled soil. The basis or source of these values is not identified.

U.S. EPA. 1993. *Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* External Review Draft. Office of Research and Development. Washington, D.C. November 1993.

This document is the source of a range of COPC enrichment ratio, *ER*, values. The recommended range, 1 to 5, has been used for organic matter, phosphorous, and other soil-bound COPCs. This document recommends a value of 3 as a "reasonable first estimate," and states that COPC enrichment occurs because lighter soil particles erode more than heavier soil particles. Lighter soil particles have higher ratios of surface area to volume and are higher in organic matter content. Therefore, concentration of organic COPCs, which is a function of the organic carbon content of sorbing media, is expected to be higher in eroded material than in in-situ soil.

This document is also a source of the following:

- A "relatively narrow range" for soil dry bulk density, *BD*, of 1.2 to 1.7 g/cm^3
- COPC-specific (inorganic COPCs only) Kd_s values used to develop a proposed range (2 to 280,000 mL/g) of Kd_s values
- A range of soil volumetric water content (θ_{sw}) values of 0.1 mL/cm^3 (very sandy soils) to 0.3 mL/cm^3 (heavy loam/clay soils) (however, no source or reference is provided for this range)

U.S. EPA. 1994. *Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities.* April 15.

U.S. EPA. 1994a. *Estimating Exposure to Dioxin-Like Compounds. Volume III: Site-specific Assessment Procedures.* External Review Draft. Office of Research and Development. Washington, D.C. EPA/600/6-88/005Cc. June.

This document is the source of values for soil mixing zone depth, Z_s, for tilled and untilled soil, as cited in U.S. EPA (1993).

U.S. EPA. 1994b. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities.* Office of Emergency and Remedial Response. Office of Solid Waste. December 14.

This document recommends (1) a default soil bulk density value of 1.5 g soil/cm^3 soil, based on a mean value for loam soil that is taken from Carsel, Parrish, Jones, Hansen, and Lamb (1988), and (2) a default soil volumetric water content, θ_{sw}, value of 0.2 mL water/cm^3 soil, based on U.S. EPA (1993).

U.S. EPA. 1998. "Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilitites." External Peer Review Draft. U.S. EPA Region 6 and U.S. EPA OSW. Volumes 1-3. EPA530-D-98-001A. July.

TABLE B-1-4

COPC LOSS CONSTANT DUE TO RUNOFF
(SOIL EQUATIONS)

(Page 1 of 5)

Description

This equation calculates the constant for COPC loss resulting from runoff of soil. Uncertainties associated with this equation include the following:

(1) For soluble COPCs, leaching might lead to movement to below 1 cm in soils and resulting in a greater mixing depth. This uncertainty may overestimate *ksr*.
(2) Deposition to hard surfaces may result in dust residues that have negligible dilution, in comparison to that of other residues. This uncertainty may underestimate *ksr*.

Equation

$$ksr = \frac{RO}{\theta_{sw} \cdot Z_s} \cdot \left(\frac{1}{1 + \left(Kd_s \cdot BD / \theta_{sw} \right)} \right)$$

Variable	Description	Units	Value
ksr	COPC loss constant due to surface runoff	yr^{-1}	
RO	Average annual surface runoff	cm/yr	**Varies (site-specific)** This variable is site-specific. According to U.S. EPA (1993; 1994b) and NC DEHNR (1997), average annual surface runoff can be estimated by using the *Water Atlas of the United States* (Geraghty, Miller, Van der Leeden, and Troise 1973). According to NC DEHNR, (1997), estimates can also be made by using more detailed, site-specific procedures for estimating the amount of surface runoff, such as those based on the U.S. Soil Conservation Service curve number equation (CNE). U.S. EPA (1985) is cited as an example of such a procedure. The following uncertainty is associated with this variable: (1) To the extent that site-specific or local average annual surface runoff information is not available, default or estimated values may not accurately represent site-specific or local conditions. As a result, *ksl* may be under- or overestimated to an unknown degree.

TABLE B-1-4

COPC LOSS CONSTANT DUE TO RUNOFF
(SOIL EQUATIONS)

(Page 2 of 5)

Variable	Description	Units	Value
θ_{sw}	Soil volumetric water content	mL/cm^3	**0.2** This variable depends on the available water and on soil structure; if a representative watershed soil can be identified, θ_{sw} can be estimated as the midpoint between a soil's field capacity and wilting point. However, U.S. EPA OSW recommends the use of 0.2 mL/cm^3 as a default value. This value is the midpoint of the range 0.1 (very sandy soils) to 0.3 (heavy loam/clay soils), which is recommended by U.S. EPA (1993) (no source or reference is provided for this range) and is consistent with U.S. EPA (1994b). The following uncertainty is associated with this variable: (1) The default θ_{sw} values may not accurately reflect site-specific or local conditions; therefore, *kse* may be under- or overestimated to a small extent, based on the limited range of values.
Z_s	Soil mixing zone depth	cm	**1 or 20** U.S. EPA OSW recommends the following values for this variable: Soil — Depth (cm) Untilled — 1 Tilled — 20 The following uncertainty is associated with this variable: (1) For soluble COPCs, leaching might lead to movement to below 1 cm in soils and justify a greater mixing depth. This uncertainty may overestimate *ksr*. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with in-situ materials), in comparison to that of other residues. This uncertainty may underestimate *ksr*.
Kd_s	Soil-water partition coefficient	cm^3/g	**Varies (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-2. The following uncertainty is associated with this variable: (1) Uncertainties associated with this parameter will be limited if Kd_s values are calculated as described in Appendix A-2.

TABLE B-1-4

COPC LOSS CONSTANT DUE TO RUNOFF
(SOIL EQUATIONS)

Variable	Description	Units	Value
BD	Soil bulk density	g/cm^3	**1.5** This variable is affected by the soil structure, such as looseness or compaction of the soil, depending on the water and clay content of the soil (Hillel 1980), as summarized by U.S. EPA 1990. A range of 0.83 to 1.84 was originally cited in Hoffman and Baes (1979). U.S. EPA (1994) recommended a default soil bulk density value of 1.5 g/cm^3, based on a mean value for loam soil that is taken from Carsel, Parrish, Jones, Hansen, and Lamb (1988). The value of 1.5 g/cm^3 also represents the midpoint of the "relatively narrow range" for *BD* of 1.2 to 1.7 g/cm^3 (U.S. EPA 1993). The following uncertainty is associated with this variable: (1) The recommended range of soil dry bulk density values may not accurately represent site-specific soil conditions.

TABLE B-1-4

COPC LOSS CONSTANT DUE TO RUNOFF (SOIL EQUATIONS)

REFERENCES AND DISCUSSION

Carsel, R.F., R.S. Parrish, R.L. Jones, J.L. Hansen, and R.L. Lamb. 1988. "Characterizing the Uncertainty of Pesticide Leaching in Agricultural Soils." *Journal of Contaminant Hydrology*. Vol. 2. Pages 11-24.

This document is cited by U.S. EPA (1994) as the source of a mean soil bulk density, *BD*, value of 1.5 g/cm^3 for loam soil.

Geraghty, J.J., D.W. Miller, F. Van der Leeden, and F.L. Troise. 1973. *Water Atlas of the United States*. Water Information Center, Port Washington, New York.

This document is cited by U.S. EPA (1993), U.S. EPA (1994c), and NC DEHNR (1997) as a reference to calculate average annual runoff, *R*. This reference provides maps with isolines of annual average surface water runoff, which is defined as all flow contributions to surface water bodies, including direct runoff, shallow interflow, and ground water recharge. Because these values are total contributions, and not only surface runoff, U.S. EPA (1994c) recommends that they be reduced by 50 percent to estimate surface runoff.

Hillel, D. 1980. Fundamentals of Soil Physics. Academic Press, Inc. New York.

This document is cited by U.S. EPA (1990) for the statement that dry soil bulk density, *BD*, is affected by the soil structure, such as looseness or compaction of the soil, depending on the water and clay content of the soil.

Hoffman, F.O., and C.F. Baes. 1979. *A Statistical Analysis of Selected Parameters for Predicting Food Chain Transport and Internal Dose of Radionuclides*. ORNL/NUREG/TM-882.

This document presents a soil bulk density, *BD*, range of 0.83 to 1.84.

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units*. January.

This document is one of the source documents that cites the use of the equation in Table B-1-4; however, this document is not the original source of this equation (this source is unknown). This document also recommends the following:

- Estimation of annual current runoff, *RO* (cm/yr), by using the *Water Atlas of the United States* (Geraghty, Miller, Van der Leeden, and Troise 1973) or site-specific procedures, such as using the U.S. Soil Conservation Service curve number equation (CNE) (U.S. EPA [1985]) is cited as an example of the use of the CNE
- Default value of 0.2 mL/cm^3 for soil volumetric water content (θ_{sw})
- Range (2 to 280,000 mL/g) of Kd_s values for inorganic COPCs (the original source of the values is not identified)

U.S. EPA. 1985. *Water Quality Assessment: A Screening Procedure for Toxic and Conventional Pollutants in Surface and Ground Water—Part I (Revised. 1985)*. Environmental Research Laboratory. Athens, Georgia. EPA/600/6-85/002a. September.

This document is cited by NC DEHNR (1997) as an example of the use of the U.S. Soil Conservation Service CNE to estimate site-specific surface runoff.

U.S. EPA. 1990. *Interim Final Methodology for Assessing Health Risks Assocated with Indirect Exposure to Combustor Emissions*. Environmental Criteria and Assessment Office. Office of Research and Development. EPA 600-90-003. January.

This document presents the statement that dry soil bulk density, *BD*, is affected by the soil structure, such as looseness or compaction of the soil, depending on the water and clay content of the soil.

U.S. EPA. 1993. *Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* External Review Draft. Office of Research and Development. Washington, D.C. November.

This document recommends the following:

- A "relatively narrow range" for soil dry bulk density, *BD*, of 1.2 to 1.7 g./cm^3
- A range of soil volumetric water content, θ_{sw}, values of 0.1 (very sandy soils) to 0.3 (heavy loam/clay soils) (the original source of, or reference for, these values is not identified)
- A range (2 to 280,000 mL/g) of Kd_s values for inorganic COPCs
- Use of the *Water Atlas of the United States* (Geraghty, Miller, Van der Leeden, and Troise 1973) to calculate average annual runoff

U.S. EPA. 1994a. *Estimating Exposure to Dioxin-Like Compounds. Volume III: Site-specific Assessment Procedures.* External Review Draft. Office of Research and Development. Washington, D.C. EPA/600/6-88/005Cc. June.

This document presents a range of values for soil mixing zone depth, Z_s, for tilled and untilled soil as cited in U.S. EPA (1993).

U.S. EPA. 1994b. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes.* Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities. Offices of Emergency and Remedial Response. Office of Solid Waste. December 14.

This document recommends the following:

- Estimation of average annual runoff, *RO*, by using the *Water Atlas of the United States* (Geraghty, Miller, Van der Leeden, and Troise 1973)
- Default soil dry bulk density, *BD*, value of 1.5 g/cm^3, based on the mean for loam soil that is taken from Carsel, Parrish, Jones, Hansen, and Lamb (1988)
- Default soil volumetric water content, θ_{sw}, value of 0.2 mL/cm^3, based on U.S. EPA (1993)

TABLE B-1-5

COPC LOSS CONSTANT DUE TO LEACHING
(SOIL EQUATIONS)

(Page 1 of 6)

Description

This equation calculates the constant for COPC loss resulting from leaching of soil. Uncertainties associated with this equation include the following:

(1) For soluble COPCs, leaching might lead to movement to below 1 or 20 cm in soils; resulting in a greater mixing depth. This uncertainty may overestimate *ksl*.
(2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with in-situ materials), in comparison to that of other residues. This uncertainty may underestimate *ksl*.
(3) The original source of this equation has not been identified. U.S. EPA (1993) presents the equation as shown here. U.S. EPA (1994) and NC DEHNR (1997) replaced the numerator as shown with "*q*", defined as average annual recharge (cm/yr).

Equation

$$ksl = \frac{P + I - RO - E_v}{\theta_{sw} \cdot Z_s \cdot \left[1.0 + \left(BD \cdot Kd_s / \theta_{sw}\right)\right]}$$

Variable	Description	Units	Value
ksl	COPC loss constant due to leaching	yr^{-1}	
P	Average annual precipitation	cm/yr	**18.06 to 164.19 (site-specific)** This variable is site-specific. This range is based on information, presented in U.S. EPA (1990), representing data for 69 selected cities (U.S. Bureau of Census 1987; Baes, Sharp, Sjoreen and Shor 1984). The 69 selected cities are not identified. However, they appear to be located throughout the continental United States. U.S. EPA OSW recommends that site-specific data be used. The following uncertainty is associated with this variable: (1) To the extent that a site is not located near an established meteorological data station, and site-specific data are not available, default average annual precipitation data may not accurately reflect site-specific conditions. As a result, *ksl* may be under- or overestimated. However, average annual precipitation data are reasonably available; therefore, uncertainty introduced by this variable is expected to be minimal.

TABLE B-1-5

COPC LOSS CONSTANT DUE TO LEACHING
(SOIL EQUATIONS)

(Page 2 of 6)

Variable	Description	Units	Value
I	Average annual irrigation	cm/yr	**0 to 100 (site-specific)** This variable is site-specific. This range is based on information, presented in U.S. EPA (1990), representing data for 69 selected cities (Baes, Sharp, Sjoreen, and Shor 1984). The 69 selected cities are not identified; however, they appear to be located throughout the continental United States. The following uncertainty is associated with this variable: (1) To the extent that site-specific or local average annual irrigation information is not available, default values (generally based on the closest comparable location) may not accurately reflect site-specific conditions. As a result, *ksl* may be under- or overestimated to an unknown degree.
RO	Average annual surface runoff	cm/yr	**Varies (site-specific)** This variable is site-specific. According to U.S. EPA (1993; 1994) and NC DEHNR (1997), average annual surface runoff can be estimated by using the Water Atlas of the United States (Geraghty, Miller, Van der Leeden, and Troise 1973). Also according to NC DEHNR (1997), this estimate can also be made by using more detailed, site-specific procedures, such as those based on the U.S. Soil Conservation Service CNE. U.S. EPA (1985) is cited as an example of such a procedure. The following uncertainty is associated with this variable: (1) To the extent that site-specific or local average annual surface runoff information is not available, default or estimated values may not accurately represent site-specific or local conditions. As a result, *ksl* may be under- or overestimated to an unknown degree.
E_v	Average annual evapotranspiration	cm/yr	**35 to 100 (site-specific)** This variable is site-specific. This range is based on information, presented in U. S. EPA (1990), representing data from 69 selected cities. The 69 selected cities are not identified; however, they appear to be located throughout the continental United States. The following uncertainty is associated with this variable: (1) To the extent that site-specific or local average annual evapotranspiration information is not available, default values may not accurately reflect site-specific conditions. As a result, *ksl* may be under- or overestimated to an unknown degree.

TABLE B-1-5

COPC LOSS CONSTANT DUE TO LEACHING
(SOIL EQUATIONS)

(Page 3 of 6)

Variable	Description	Units	Value
θ_{sw}	Soil volumetric water content	mL/cm^3	**0.2** This variable depends on the available water and on soil structure. θ_{sw} can be estimated as the midpoint between a soil's field capacity and wilting point, if a representative watershed soil can be identified. However, U.S. EPA OSW recommends the use of 0.2 mL/cm^3 as a default value. This value is the midpoint of the range of 0.1 (very sandy soils) to 0.3 (heavy loam/clay soils) recommended by U.S. EPA (1993) (no source or reference is provided for this range) and is consistent with U.S. EPA (1994). The following uncertainty is associated with this variable: (1) The default θ_{sw} values may not accurately reflect site-specific or local conditions; therefore, *ksl* may be under- or overestimated to a small extent, based on the limited range of values.
Z_s	Soil mixing zone depth	cm	**1 or 20** U.S. EPA OSW recommends the following values for this variable: Soil — Depth (cm) Untilled — 1 Tilled — 20 Uncertainties associated with this variable include the following: (1) For soluble COPCs, leaching might lead to movement to below 1 or 20 cm in soils; resulting in a greater mixing depth. This uncertainty may overestimate *ksl*. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution, in comparison to that of other residues. This uncertainty may underestimate *ksl*.

TABLE B-1-5

COPC LOSS CONSTANT DUE TO LEACHING
(SOIL EQUATIONS)

Variable	Description	Units	Value
BD	Soil bulk density	g/cm^3	**1.5** This variable is affected by the soil structure, such as looseness or compaction of the soil, depending on the water and clay content of the soil (Hillel 1980), as summarized in U.S. EPA (1990). A range of 0.83 to 1.84 was originally cited in Hoffman and Baes (1979). U.S. EPA (1994) recommended a default soil bulk density value of 1.5 g/cm^3, based on a mean value for loam soil from Carsel, Parrish, Jones, Hansen, and Lamb (1988). The value of 1.5 g/cm^3 also represents the midpoint of the "relatively narrow range" for *BD* of 1.2 to 1.7 g/cm^3 (U.S. EPA 1993). The following uncertainties is associated with this variable: (1) The recommended range of soil dry bulk density values may not accurately represent site-specific soil conditions.
Kd_s	Soil-water partition coefficient	cm^3/g	**Varies (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-2. The following uncertainty is associated with this variable: (1) Uncertainties associated with this parameter will be limited if Kd_s values are calculated as described in Appendix A-2.

TABLE B-1-5

COPC LOSS CONSTANT DUE TO LEACHING (SOIL EQUATIONS)

REFERENCES AND DISCUSSION

Baes, C.F., R.D. Sharp, A.L. Sjoreen and R.W. Shor. 1984. "A Review and Analysis of Parameters for Assessing Transport of Environmentally Released Radionuclides through Agriculture." Prepared for the U.S. Department of Energy under Contract No. DEAC05-840R21400.

For the continental United States, as cited in U.S. EPA (1990), this document is the source of a series of maps showing: (1) average annual precipitation (*P*); (2) average annual irrigation (*I*); and (3) average annual evapotranspiration isolines.

Carsel, R.F., R.S. Parrish, R.L. Jones, J.L. Hansen, and R.L. Lamb. 1988. "Characterizing the Uncertainty of Pesticide Leaching in Agricultural Soils." *Journal of Contaminant Hydrology*. Vol. 2. Pages 11-24.

This document is cited by U.S. EPA (1994b) as the source for a mean soil bulk density value of 1.5 g/cm^3 for loam soil.

Geraghty, J.J., D.W. Miller, F. Van der Leeden, and F.L. Troise. 1973. *Water Atlas of the United States*. Water Information Center, Port Washington, New York.

This document is cited by U.S. EPA (1993), U.S. EPA (1994), and NC DEHNR (1997) as a reference for calculating average annual runoff, *RO*. This document provides maps with isolines of annual average surface runoff, which is defined as all flow contributions to surface water bodies, including direct runoff, shallow interflow, and ground water recharge. Because these volumes are total contributions—and not only surface runoff—U.S. EPA (1994) notes that they need to be reduced by 50 percent to estimate average annual surface runoff.

This document presents a soil bulk density, *BD*, range of 0.83 to 1.84. U.S. EPA has not completed its review of this document.

Hillel, D. 1980. *Fundamentals of Soil Physics*. Academic Press, Inc. New York, New York.

This document is cited by U.S. EPA (1990) for the statement that dry soil bulk density, *BD*, is affected by the soil structure, such as looseness or compaction of the soil, depending on the water and clay content of the soil.

Hoffman, F.O., and C.F. Baes. 1979. *A Statistical Analysis of Selected Parameters for Predicting Food Chain Transport and Internal Dose of Radionuclides*. ORNL/NUREG/TM-882.

This document presents a soil bulk density, *BD*, range of 0.83 to 1.84.

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units*. January.

This document is one of the source documents that cites the use of the equation in Table B-1-5; however, the document is not the original source of this equation. This document also recommends the following:

- Estimation of average annual surface runoff, *RO* (cm/yr), by using the *Water Atlas of the United States* (Geraghty, Miller, Van der Leeden, and Troise 1973) or site-specific procedures, such as using the U.S. Soil Conservation Service CNE; U.S. EPA 1985 is cited as an example of the use of the CNE.

- A default value of 0.2 mL/cm^3 for soil volumetric water content, θ_{sw}.
- A range (2 to 280,000 mL/g) of Kd_s values for inorganic COPCs; the original source of these values is not identified.

U.S. Bureau of the Census. 1987. *Statistical Abstract of the United States:* 1987. 107th edition. Washington, D.C.

This document is a source of average annual precipitation (*P*) information for 69 selected cites, as cited in U.S. EPA (1990); these 69 cities are not identified.

U.S. EPA. 1985. *Water Quality Assessment: A Screening Procedure for Toxic and Conventional Pollutants in Surface and Groundwater*. Part I (Revised 1985). Environmental Research Laboratory. Athens, Georgia. EPA/600/6-85/002a. September.

This document is cited by NC DEHNR (1997) as an example of the use of the U.S. Soil Conservation Service CNE to estimate site-specific average annual surface runoff.

U.S. EPA. 1990. *Interim Final Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. Environmental Criteria and Assessment Office. Office of Research and Development. EPA 600-90-003. January.

This document presents ranges of (1) average annual precipitation, (2) average annual irrigation, and (3) average annual evapotranspiration. This document identifies Baes, Sharp, Sjoreen, and Shor (1984) and U.S. Bureau of the Census (1987) as the original sources of this information.

U.S. EPA. 1993. *Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. External Review Draft. Office of Research and Development. Washington, D.C. November.

This document is one of the reference sources for the equation in Table B-1-5; this document also recommends the following:

- A range of soil volumetric water content, θ_{sw}, values of 0.1 (very sandy soils) to 0.3 (heavy loam/clay soils); the original source or reference for these values is not identified.
- A range (2 to 280,000 mL/g) of Kd_s values for inorganic COPCs
- A "relatively narrow range" for soil dry bulk density, *BD*, of 1.2 to 1.7 g/cm^3

This document is one of the reference source documents for equation in Table B-1-5. The original source of this equation is not identified.

U.S. EPA. 1994. *Review Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. Office of Emergency and Remedial Response. Office of Solid Waste. December 14.

This document recommends (1) a default soil volumetric water content, θ_{sw}, value of 0.2 mL/cm^3, based on U.S. EPA (1993), and (2) a default soil bulk density, *BD*, value of 1.5 g/cm^3, based on a mean value for loam soil from Carsel, Parrish, Jones, Hansen, and Lamb (1988).

TABLE B-1-6

COPC LOSS CONSTANT DUE TO VOLATILIZATION (SOIL EQUATIONS)

Description

This equation calculates the COPC loss constant from soil due to volatilization, and was obtained from *Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions* (U.S. EPA In Press). The soil loss constant due to volatilization (*ksv*) is based on gas equilibrium coefficients and gas phase mass transfer. The first order decay constant, *ksv*, is obtained by adapting the Hwang and Falco equation for soil vapor phase diffusion (Hwang and Falco 1986).

Uncertainties associated with this equation include the following:

(1) For soluble COPCs, leaching might lead to movement to below 1 centimeter in untilled soils, resulting in a greater mixing depth. This uncertainty may overestimate *ksv*.
(2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with *in situ* materials) in comparison to that of other residues. This uncertainty may underestimate *ksv*.

Equation

$$ksv = \left[\frac{3.1536 \times 10^{7} \cdot H}{Z_s \cdot Kd_s \cdot R \cdot T_a \cdot BD}\right] \cdot \left(\frac{D_a}{Z_s}\right) \cdot \left[1 - \left(\frac{BD}{\rho_s}\right) - \theta_{sw}\right]$$

Variable	Definition	Units	Value
ksv	COPC loss constant due to volatilization	yr^{-1}	
3.1536 x 10^7	Units conversion factor	s/yr	
H	Henry's Law constant	atm-m^3/mol	**Varies (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-2. The following uncertainty is associated with this variable: (1) Values for this variable, estimated by using the parameters and algorithms in Appendix A-2, may under- or overestimate the actual COPC-specific values. As a result, *ksv* may be under- or overestimated.

TABLE B-1-6

COPC LOSS CONSTANT DUE TO VOLATILIZATION
(SOIL EQUATIONS)

Variable	Definition	Units	Value
Z_s	Soil mixing zone depth	cm	**1 or 20** U.S. EPA OSW recommends the following values for this variable: Soil — Depth (cm) Untilled — 1 Tilled — 20 The following uncertainty is associated with this variable: (1) For soluble COPCs, leaching might lead to movement to below 1 or 20 cm in soils and justify a greater mixing depth. This uncertainty may overestimate *ksv*. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution, in comparison to that of other residues. This uncertainty may underestimate *ksv*.
Kd_s	Soil-water partition coefficient	cm^3/g	**Varies (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-2. The following uncertainty is associated with this variable: (1) Uncertainties associated with this parameter will be limited if Kd_s values are calculated as described in Appendix A-2.
R	Universal gas constant	atm-m^3/mol-K	**8.205×10^{-5}** There are no uncertainties associated with this parameter.
T_a	Ambient air temperature	K	**298** This variable is site-specific. U.S. EPA (1990) recommended an ambient air temperature of 298 K. The following uncertainty is associated with this variable: (1) To the extent that site-specific or local values for the variable are not available, default values may not accurately represent site-specific conditions. The uncertainty associated with the selection of a single value from within the temperature range at a single location is expected to be more significant than the uncertainty associated with choosing a single ambient temperature to represent all localities.

TABLE B-1-6

COPC LOSS CONSTANT DUE TO VOLATILIZATION
(SOIL EQUATIONS)

Variable	Definition	Units	Value
BD	Soil bulk density	g/cm^3	**1.5** This variable is affected by the soil structure, such as looseness or compaction of the soil, depending on the water and clay content of the soil (Hillel 1980; Miller and Gardiner 1998), as summarized in U.S. EPA (1990). A range of 0.83 to 1.84 was originally cited in Hoffman and Baes (1979). U.S. EPA (1994) recommended a default soil bulk density value of 1.5 g/cm^3, based on a mean value for loam soil from Carsel, Parrish, Jones, Hansen, and Lamb (1988). The value of 1.5 g/cm^3 also represents the midpoint of the "relatively narrow range" for *BD* of 1.2 to 1.7 g/cm^3 (U.S. EPA 1993). The following uncertainty is associated with this variable: (1) The recommended range of soil bulk density values may not accurately represent site-specific soil conditions.
ρ_s	Solids particle density	g/cm^3	**2.7** U.S. EPA OSW recommends the use of this value, based on Blake and Hartage (1996) and Hillel (1980). The solids particle density will vary with location and soil type.
D_a	Diffusivity of COPC in air	cm^2/s	**Varies (see Appendix A-2)** This value is COPC-specific and should be determined from the COPC tables presented in Appendix A-2. The following uncertainty is associated with this variable: (1) The default D_a values may not accurately represent the behavior of COPCs under site-specific conditions. However, the degree of uncertainty is expected to be minimal.

TABLE B-1-6

COPC LOSS CONSTANT DUE TO VOLATILIZATION
(SOIL EQUATIONS)

Variable	Definition	Units	Value
θ_{sw}	Soil volumetric water content	mL/cm^3	**0.2** This variable depends on the available water and on soil structure. θ_{sw} can be estimated as the midpoint between a soil's field capacity and wilting point, if a representative watershed soil can be identified. However, U.S. EPA OSW recommends the use of 0.2 mL/cm^3 as a default value. This value is the midpoint of the range of 0.1 (very sandy soils) to 0.3 (heavy loam/clay soils) recommended by U.S. EPA (1993) (no source or reference is provided for this range) and is consistent with U.S. EPA (1994). The following uncertainty is associated with this variable: (1) The default θ_{sw} values may not accurately reflect site-specific or local conditions; therefore, *ksl* may be under- or overestimated to a small extent, based on the limited range of values.

TABLE B-1-6

COPC LOSS CONSTANT DUE TO VOLATILIZATION (SOIL EQUATIONS)

(Page 5 of 6)

REFERENCES AND DISCUSSION

Blake, G.R. and K.H. Hartge. 1996. *Particle Density. Methods of Soil Analysis, Part 1: Physical and Mineralogical Methods*. Second Edition. Arnold Klute, Ed. American Society of Agronomy, Inc. Madison, WI., p. 381.

Carsel, R.F., R.S, Parrish, R.L. Jones, J.L. Hansen, and R.L. Lamb. 1988. "Characterizing the Uncertainty of Pesticide Leaching in Agricultural Soils." *Journal of Contaminant Hydrology*. Vol. 2. Pages 11-24.

This document is cited by U.S. EPA (1994) as the source of a mean soil bulk density value, *BD*, of 1.5 g/cm^3 for loam soil.

Hillel, D. 1980. *Fundamentals of Soil Physics.* Academic Press, Inc. New, New York.

Hoffman, F.O., and C.F. Baes. 1979. *A Statistical Analysis of Selected Parameters for Predicting Food Chain Transport and Internal Dose of Radionuclides.* ORNL/NUREG/TM-882.

This document presents a soil bulk density, *BD*, range of 0.83 to 1.84.

Hwang S. T. and Falco, J. W. 1986. "Estimation of multimedia exposures related to hazardous waste facilities", In: *Pollutants in a Multimedia Environment*. Yoram Cohen, Ed. Plenum Publishing Corp. New York.

Miller, R.W. and D.T. Gardiner. 1998. In: *Soils in Our Environment*. J.U. Miller, Ed. Prentice Hall. Upper Saddle River, NJ. pp. 80-123.

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units.* January.

This document is one of the source documents that cites the use of the equation in Table B-1-6; however, the original source of this equation is not identified. This document also recommends the following:

- A range of COPC-specific Henry's Law Constant (atm-m^3/mol) values
- A range (2 to 280,000 mL/g) of Kd_s values for inorganic COPCs; however, the sources of these values are not identified.
- A range (9.2 E-06 to 2.8 E-01 cm^2/sec) of values for diffusivity of COPCs in air; however, the sources of these values are not identified.

U. S. EPA. 1990. *Interim Final Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Environmental Criteria and Assessment Office. Office of Research and Development. EPA 600-90-003. January.

This document recommends the following:

- A default ambient air temperature of 298 K

- An average annual wind speed of 3.9 m/s; however, no source or reference for this value is identified.

U.S. EPA. 1993. *Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* External Review Draft. Office of Research and Development. Washington, D.C. November.

This document is one of the reference source documents for the equation in Table B-1-6; however, the original reference for this equation is not identified.

This document also presents the following:

- COPC-specific Kd_s values that were used to establish a range (2 to 280,000 mL/g) of Kd_s values for inorganic COPCs
- a "relatively narrow range" for soil dry bulk density, *BD*, of 1.2 to 1.7 g/cm^3

U.S. EPA. 1994. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Waste. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. Office of Emergency and Remedial Response. Office of Solid Waste. December 14.

This document recommends a default soil density, *BD*, value of 1.5 g/cm^3, based on a mean value for loam soil that is taken from Carsel, Parrish, Jones, Hansen, and Lamb (1988).

U.S. EPA. 1994b. *Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities.* April 15.

U.S. EPA. 1998. "Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilitites." External Peer Review Draft. U.S. EPA Region 6 and U.S. EPA OSW. Volumes 1-3. EPA530-D-98-001A. July.

U.S. EPA. In Press. "*Methodology for Assessing Health Risks Associated with Multiple Exposure Pathways to Combustor Emissions*." Internal Review Draft. Environmental Criteria and Assessment Office. ORD. Cincinnati, Ohio.

TABLE B-2-1

TOTAL COPC LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

(Page 1 of 4)

Description

This equation calculates the total average water body load from wet and dry vapor and particle deposition, runoff, and erosion loads.

The limitations and uncertainties incorporated by using this equation include the following:

(1) The greatest uncertainties are associated with the site-specific variables in Tables B-2-2, B-2-3, B-2-4, B-2-5, and B-2-6 (used to estimate values for the variables in the below equation for L_T). These variables include Q, $Dywwv$, $Dytwp$, A_w, $Cywv$, A_I, A_L, Cs, and X_e. Values for many of these variables are estimated through the use of mathematical models and the uncertainties associated with values for these variables may be significant in some cases.

(2) Uncertainties associated with the remaining variables in Tables B-2-2, B-2-3, B-2-4, B-2-5, and B-2-6 are expected to be less significant, primarily because of the narrow ranges of probable values for these variables or because values for these variables (such as Kd_s) were estimated by using well-established estimation methods.

Equation

$$L_T = L_{DEP} + L_{Dif} + L_{RI} + L_R + L_E$$

Variable	Description	Units	Value
L_T	Total COPC load to the water body	g/yr	
L_{DEP}	Total (wet and dry) particle phase and wet vapor phase direct deposition load to water body	g/yr	**Varies (calculated - Table B-2-2)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-2. Uncertainties associated with this variable include the following: (1) Most of the uncertainties associated with the variables in Table B-2-2, specifically those associated with Q, $Dywwv$, $Dytwp$, and A_w, are site-specific and may be significant in some cases.

TABLE B-2-1

TOTAL COPC LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
L_{Dif}	Vapor phase COPC diffusion (dry deposition) load to water body	g/yr	**Varies (calculated - Table B-2-3)** This variable is calculated by using the equation in Table B-2-3. Uncertainties associated with this variable include the following: (1) Most of the uncertainties associated with the variables in the equation in Table B-2-3, specifically those associated with *Q*, *Cywv*, and A_W, are site-specific and may be significant in some cases.
L_{RI}	Runoff load from impervious surfaces	g/yr	**Varies (calculated - Table B-2-4)** This variable is calculated by using the equation in Table B-2-4. Uncertainties associated with this variable include the following: (1) Most of the uncertainties associated with the variables in this equation, specifically those associated with *Q*, *Dywwv*, *Dytwp*, and A_I, are site-specific.
L_R	Runoff load from pervious surfaces	g/yr	**Varies (calculated - Table B-2-5)** This variable is calculated by using the equation in Table B-2-5. Uncertainties associated with this variable include the following: (1) Most of the uncertainties associated with the variables in the equation in Table B-2-5, specifically those for A_L, A_I, and *Cs*, are site-specific and may be significant in some cases. (2) Uncertainties associated with the remaining variable in the equation in Table B-2-5 are not expected to be significant, primarily because of the narrow ranges of probable values for these variables or the use of well-established estimation procedures (Kd_s).

TABLE B-2-1

TOTAL COPC LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
L_E	Soil erosion load	g/yr	**Varies (calculated - Table B-2-6)** This variable is calculated by using the equation in Table B-2-6. Uncertainties associated with this variable include the following: (1) Most of the uncertainties associated with the variables in the equation in Table B-2-6, specifically those for X_e, A_L, A_I, and Cs, are site-specific and may be significant in some cases. (2) Uncertainties associated with the remaining variables in the equation in Table B-2-6 are not expected to be significant, primarily because of the narrow range of probable values for these variables or the use of well-established estimation procedures (Kd_s).

TABLE B-2-1

TOTAL COPC LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

REFERENCES AND DISCUSSION

Bidleman, T.F. 1988. "Atmospheric Processes." *Environmental Science and Technology*. Volume 22. Number 4. Pages 361-367.

For discussion, see References and Discussion in Table B-1-1.

TABLE B-2-2

DEPOSITION TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

Description

This equation calculates the average load to the water body from direct deposition of wet and dry particles and wet vapors onto the surface of the water body.

Uncertainties associated with this equation include the following:

(1) Most of the uncertainties associated with the variables in this equation, specifically those associated with *Q, Dywwv, Dytwp* , and A_W.
(2) It is calculated on the basis of the assumption of a default S_T value for background plus local sources, rather than an S_T value for urban sources. If a specific site is located in an urban area, the use of the latter S_T value may be more appropriate. Specifically, the S_T value for urban sources is about one order of magnitude greater than that for background plus local sources and would result in a lower calculated F_v value; however, the F_v value is likely to be only a few percent lower.

Equation

$$L_{DEP} = Q \bullet [F_v \bullet Dywwv + (1 - F_v) \bullet Dytwp] \bullet A_W$$

For mercury modeling:

$$L_{DEP_{Mercury}} = 0.48 Q_{TotalMercury} \cdot [F_{v_{Hg^{2+}}} \cdot Dywwv + (1 - F_{v_{Hg^{2+}}}) \cdot Dytwp] \cdot A_w$$

In calculating L_{DEP} for mercury comounds, L_{DEP}*(Mercury)* is calculated as shown above using the total mercury emission rate (Q) measured at the stack and F_v for mercuric chloride (F_v = 0.85). As presented below, the calculated L_{DEP}*(Mercury)* value is apportioned into the divalent mercury (Hg^{2+}) and methyl mercury (MHg) forms based on a 85% Hg^{2+} and 15% MHg speciation split in the water body (see Chapter 2).

$L_{DEP}(Hg^{2+})$ = 0.85 L_{DEP} *Mercury*
L_{DEP}(MHg) = 0.15 L_{DEP} *Mercury*

After calculating species specific L_{DEP} values, divalent and methyl mercury should continue to be modeled throughout Appendix B equations as individual COPCs.

Variable	Description	Units	Value
L_{DEP}	Total (wet and dry) particle-phase and wet vapor phase direct deposition load to water body	g/yr	

TABLE B-2-2

DEPOSITION TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

(Page 2 of 3)

Variable	Description	Units	Value
Q	COPC-specific emission rate	g/s	**Varies (site-specific)** This variable is COPC- and site-specific (see Chapters 2 and 3). Uncertainties associated with this variable are site-specific.
F_v	Fraction of COPC air concentration in vapor phase	unitless	**0 to 1 (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-2. Uncertainties associated with this variable include the following: (1) It is based on the assumption of a default S_T value for background plus local sources, rather than an S_T value for urban sources. If a specific site is located in an urban area, the use of the latter S_T value may be more appropriate. Specifically, the S_T value for urban sources is about one order of magnitude greater than that for background plus local sources and would result in a lower calculated F_v value; however, the F_v value is likely to be only a few percent lower. (2) According to Bidleman (1988), the equation used to calculate F_v assumes that the variable c (Junge constant) is constant for all chemicals; however, the value of c depends on the chemical (sorbate) molecular weight, the surface concentration for monolayer coverage, and the difference between the heat of desorption from the particle surface and the heat of vaporization of the liquid-phase sorbate. To the extent that site- or COPC-specific conditions may cause the value of c to vary, uncertainty is introduced if a constant value of c is used to calculate F_v.
Dywwv	Unitized yearly average wet deposition from vapor phase (over water body)	s/m^2-yr	**Varies (modeled)** This variable is COPC- and site-specific, and is determined by air dispersion modeling (see Chapter 3). Uncertainties associated with this variable are site-specific.
Dytwp	Unitized yearly average total (wet and dry) deposition from particle phase (over water body)	s/m^2-yr	**Varies (modeled)** This variable is COPC- and site-specific, and is determined by air dispersion modeling (see Chapter 3). Uncertainties associated with this variable are site-specific.
A_W	Water body surface area	m^2	**Varies (modeled)** This variable is COPC- and site-specific (see Chapter 4). Uncertainties associated with this variable are site-specific.

TABLE B-2-2

DEPOSITION TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

REFERENCES AND DISCUSSION

Bidleman, T.F. 1988. "Atmospheric Processes." *Environmental Science and Technology*. Volume 22. Number 4. Pages 361-367.

Junge, C.E. 1977. *Fate of Pollutants in Air and Water Environments, Part I*. Suffet, I.H., Ed. Wiley. New York. Pages 7-26.

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units.* January.

This document is a reference source for the equation in B-2-2. This document also recommends by using the equations in Bidleman (1988) to calculate F_v values for all organics other than dioxins (PCDD/PCDFs). However, the document does not present a recommendation for dioxins. Finally, this document states that metals are generally entirely in the particulate phase ($F_v = 0$) except for mercury, which is assumed to be entirely in the vapor phase. The document does not state whether F_v for mercury should be calculated by using the equations in Bidleman (1988).

U.S. EPA. 1994. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities.* Office of Emergency and Remedial Response. Office of Solid Waste. December 14.

This document is a reference source for the equation in Table B-2-2. This document also presents values for organic COPCs that range from 0.27 to 1. F_v values for organics other than PCDD/PCDFs are calculated by using the equations presented in Bidleman (1988). The F_v value for PCDD/PCDFs is assumed to be 0.27, based on U.S. EPA (no date). Finally, this document presents F_v values for inorganic COPCs equal to 0, based on the assumption that these COPCs are nonvolatile and assumed to be 100 percent in the particulate phase and 0 percent in the vapor phase.

TABLE B-2-3

DIFFUSION LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

Description

This equation calculates the load to the water body due to dry vapor diffusion. Uncertainties associated with this equation include the following:

(1) Most of the uncertainties associated with the variables in this equation, specifically those associated with K_v, Q, Cyv, and A_w, are site-specific.
(2) This equation assumes a default S_T value for background plus local sources, rather than an S_T value for urban sources. If a specific site is located in an urban area, the use of the latter S_T value may be more appropriate. Specifically, the S_T value for urban sources is about one order of magnitude greater than that for background plus local sources and would result in a lower calculated F_v value; however, the F_v value is likely to be only a few percent lower.

Equation

$$L_{Dif} = \frac{K_v \cdot Q \cdot F_v \cdot Cywv \cdot A_W \cdot 1.0\times10^{-6}}{\frac{H}{R \cdot T_{wk}}}$$

For mercury modeling:

$$L_{Dif_{Mercury}} = \frac{K_{v_{Hg^{2+}}} \cdot 0.48Q_{TotalMercury} \cdot F_{v_{Hg^{2+}}} \cdot Cywv \cdot A_w \cdot 1.0\times10^{-06}}{\frac{H_{Hg^{2+}}}{R \cdot T_{wk}}}$$

In calculating L_{Dif} for mercury comounds, L_{Dif}*(Mercury)* is calculated as shown above using the total mercury emission rate (Q) measured at the stack and F_v for mercuric chloride (F_v = 0.85). As presented below, the calculated L_{Dif}*(Mercury)* value is apportioned into the divalent mercury (Hg^{2+}) and methyl mercury (MHg) forms based on a 85% Hg^{2+} and 15% MHg speciation split in the water body (see Chapter 2).

$L_{Dif}(Hg^{2+})$ = 0.85 L_{Dif} *Mercury*
L_{Dif}(MHg) = 0.15 L_{Dif} *Mercury*

After calculating species specific L_{Dif} values, divalent and methyl mercury should continue to be modeled throughout Appendix B equations as individual COPCs.

TABLE B-2-3

DIFFUSION LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

(Page 2 of 4)

Variable	Description	Units	Value
L_{Dif}	Dry vapor phase diffusion load to water body	g/yr	
K_v	Overall transfer rate coefficient	m/yr	**Varies (calculated - Table 2-13)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-13.
Q	COPC-specific emission rate	g/s	**Varies (site-specific)** This variable is COPC- and site-specific (see Chapters 2 and 3). Uncertainties associated with this variable are site--specific.
F_v	Fraction of COPC air concentration in vapor phase	unitless	**0 to 1 (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-2. Uncertainties associated with this variable include the following: (1) This equation assumes a default S_T value for background plus local sources, rather than an S_T value for urban sources. If a specific site is located in an urban area, the use of the latter S_T value may be more appropriate. Specifically, the S_T value for urban sources is about one order of magnitude greater than that for background plus local sources and would result in a lower calculated F_v value; however, the F_v value is likely to be only a few percent lower. (2) According to Bidleman (1988), the equation used to calculate F_v assumes that the variable c is constant for all chemicals; however, the value of c depends on the chemical (sorbate) molecular weight, the surface concentration for monolayer coverage, and the difference between the heat of desorption from the particle surface and the heat of vaporization of the liquid-phase sorbate. To the extent that site- or COPC-specific conditions may cause the value of c to vary, uncertainty is introduced if a constant value of c issued to calculate F_v.
Cywv	Unitized yearly average air concentration from vapor phase (over water body)	µg-s/g-m^3	**Varies (modeled)** This variable is COPC- and site-specific, and is determined for each water body by air dispersion modeling (see Chapter 3). Uncertainties associated with this variable are site-specific.

TABLE B-2-3

DIFFUSION LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

(Page 3 of 4)

Variable	Description	Units	Value
A_W	Water body surface area	m^2	**Varies (site-specific)** This variable is site-specific (see Chapter 4). Uncertainties associated with this variable are site-specific. However, it is expected that the uncertainty associated with this variable will be limited, because maps, aerial photographs, and other resources from which water body surface areas can be measured, are readily available.
H	Henry's Law constant	atm-m^3/mol	**Varies (see Appendix A-2)** This variable is COPC-specific, and should be determined from the COPC tables in Appendix A-2. The following uncertainty is associated with this variable: (1) Values for this variable, estimated by using the parameters and algorithms in Appendix A-2, may under- or overestimate the actual COPC-specific values. As a result, L_{Dif} may be under- or overestimated to a limited degree.
R	Universal gas constant	atm-m^3/mol-K	**8.205×10^{-5}**
T_{wk}	Water body temperature	K	**298** This variable is site-specific. U.S. EPA OSW recommends the use of this default value in the absence of site-specific information, consistent with U.S. EPA (1993 and 1994). The following uncertainty is associated with this variable: (1) To the extent that the default water body temperature value does not accurately represent site-specific or local conditions, L_{Dif} will be under- or overestimated.

TABLE B-2-3

DIFFUSION LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

REFERENCES AND DISCUSSION

Bidleman, T.F. 1988. *"Atmospheric Processes." Environmental Science and Technology.* Volume 22. Number 4. Pages 361-367.

NC DEHNR. 1997. NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units. January.

This document is a reference source for the equation in Table B-2-3. This document also recommends using the equations in Bidleman (1988) to calculate F_v values for all organics other than dioxins (PCDD/PCDFs).

U.S. EPA. 1993. *Addendum to Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* External Review Draft. Office of Solid Waste and Office Research and Development. Washington, D.C. November 10.

This document recommends a range (10°C to 30°C, 283 K to 303 K) for water body temperature, T_{wk}. No source was identified for this range.

U.S. EPA 1994. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities.* Office of Emergency and Remedial Response. Office of Solid Waste. December 14.

This document is cited as the reference source for $T_{wk,}$ water body temperature (298 K); however, no references or sources are identified for this value. This document is a reference source for the equation in Table B-2-2.

TABLE B-2-4

IMPERVIOUS RUNOFF LOAD TO WATER BODY (SURFACE WATER AND SEDIMENT EQUATIONS)

Description

This equation calculates the average runoff load to the water body from impervious surfaces in the watershed from which runoff is conveyed directly to the water body.

Uncertainties associated with this equation include the following:

(1) Most of the uncertainties associated with the variables in this equation, specifically those associated with *Q*, *Dywwv*, *Dytwp*, and A_I, are site-specific.
(2) The equation assumes a default S_T value for background plus local sources, rather than an S_T value for urban sources. If a specific site is located in an urban area, the use of the latter S_T value may be more appropriate. Specifically, the S_T value for urban sources is about one order of magnitude greater than that for background plus local sources and would result in a lower calculated F_v value; however, the F_v value is likely to be only a few percent lower.

Equation

$$L_{RI} = Q \cdot \left[F_v \cdot Dywwv + (1 - F_v) \cdot Dytwp \right] \cdot A_I$$

For mercury modeling:

$$L_{RI_{Mercury}} = 0.48 Q_{TotalMercury} \cdot \left[F_{v_{Hg^{2+}}} \cdot Dywwv + (1.0 - F_{v_{Hg^{2+}}}) \cdot Dytwp \right] \cdot A_I$$

In calculating L_{RIP} for mercury comounds, L_{RI}*(Mercury)* is calculated as shown above using the total mercury emission rate (*Q*) measured at the stack and F_v for mercuric chloride (F_v = 0.85). As presented below, the calculated L_{RI}*(Mercury)* value is apportioned into the divalent mercury (Hg^{2+}) and methyl mercury (MHg) forms based on a 85% Hg^{2+} and 15% MHg speciation split in the water body (see Chapter 2).

$L_{RI}(Hg^{2+})$ = 0.85 L_{RI} *Mercury*
L_{RI}(MHg) = 0.15 L_{RI} *Mercury*

After calculating species specific L_{RI} values, divalent and methyl mercury should continue to be modeled throughout Appendix B equations as individual COPCs.

TABLE B-2-4

IMPERVIOUS RUNOFF LOAD TO WATER BODY (SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
L_{RI}	Runoff load from impervious surfaces	g/yr	
Q	COPC-specific emission rate	g/s	**Varies (site-specific)** This variable is COPC- and site-specific, and is determined by air dispersion modeling (see Chapters 2 and 3). Uncertainties associated with this variable are site-specific.
F_v	Fraction of COPC air concentration in vapor phase	unitless	**0 to 1 (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-2. Uncertainties associated with this variable include the following: (1) The equation assumes a default S_T value for background plus local sources, rather than an S_T value for urban sources. If a specific site is located in an urban area, the use of the latter S_T value may be more appropriate. Specifically, the S_T value for urban sources is about one order of magnitude greater than that for background plus local sources and would result in a lower calculated F_v value; however, the F_v value is likely to be only a few percent lower. (2) According to Bidleman (1988), the equation used to calculate F_v assumes that the variable c is constant for all chemicals; however, the value of c depends on the chemical (sorbate) molecular weight, the surface concentration for monolayer coverage, and the difference between the heat of desorption from the particle surface and the heat of vaporization of the liquid-phase sorbate. To the extent that site- or COPC-specific conditions may cause the value of c to vary, uncertainty is introduced if a constant value of c is used to calculate F_v.
Dywwv	Unitized yearly average wet deposition from vapor phase (over watershed)	s/m^2-yr	**Varies (modeled)** This variable is COPC- and site-specific, and is determined by air dispersion modeling (see Chapter 3). Uncertainties associated with this variable are site-specific.
Dytwp	Unitized yearly average total (wet and dry) deposition from particle phase (over watershed)	s/m^2-yr	**Varies (modeled)** This variable is COPC- and site-specific, and is determined by air dispersion modeling (see Chapter 3). Uncertainties associated with this variable are site-specific.
A_I	Impervious watershed area receiving COPC deposition	m^2	**Varies (site-specific)** This variable is COPC- and site-specific. Uncertainties associated with this variable are site-specific.

TABLE B-2-4

IMPERVIOUS RUNOFF LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

REFERENCES AND DISCUSSION

Bidleman, T.F. 1988. "Atmospheric Processes." *Environmental Science and Technology.* Volume 22. Number 4. Pages 361-367.

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units.* January.

This document is a reference source for the equation in Table B-2-4. This document also recommends using the equations in Bidleman (1988) to calculate F_v values for all organics other than dioxins (PCDD/PCDFs). However, the document does not present a recommendation for dioxins. Finally, this document states that metals are generally entirely in the particulate phase ($F_v = 0$) except for mercury, which is assumed to be entirely in the vapor phase. The document does not state whether F_v for mercury should be calculated by using the equations in Bidleman (1988).

U.S. EPA. 1994. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. Office of Emergency and Remedial Response. Office of Solid Waste. December 14.

This document is a reference source for the equation in Table B-2-4.

TABLE B-2-5

PERVIOUS RUNOFF LOAD TO WATER BODY (SURFACE WATER AND SEDIMENT EQUATIONS)

Description

This equation calculates the average runoff load to the water body from pervious soil surfaces in the watershed.

Uncertainties associated with this equation include the following:

(1) To the extent that site-specific or local average annual surface runoff information is not available, default or estimated values may not accurately represent site-specific or local conditions. As a result, L_R may be under- or overestimated to an unknown degree.
(2) The recommended range of soil bulk density values may not accurately represent site-specific soil conditions; specifically, this range may under- or overestimate site-specific soil conditions to an unknown degree.
(3) The default θ_{sw} values may not accurately reflect site-specific or local conditions; therefore, L_R may be under- or overestimated to a small extent, based on the limited range of values.
(4) Various uncertainties are associated with *Cs*; see the equation in Table B-1-1.

Equation

$$L_R = RO \cdot \left(A_L - A_I\right) \cdot \frac{Cs \cdot BD}{\theta_{sw} + Kd_s \cdot BD} \cdot 0.01$$

For mercury modeling:

For mercury modeling, $L_{R\,(Initial)}$ values are calculated for divalent mercury (Hg^{2+}) and methyl mercury (MHg) using their respective *Cs* and Kd_s values; then as indicated below, these values are apportioned based on a 85% Hg^{2+} and 15% MHg speciation split in the water body (see Chapter 2).

$$L_{R_{Hg^{2+}}} = L_{R_{Hg^{2+}\,(Initial)}} \cdot 0.85$$

$$L_{R_{MHg}} = L_{R_{MHg\,(Initial)}} + (L_{R_{Hg^{2+}\,(Initial)}} \cdot 0.15)$$

After calculating species specific L_R values, divalent and methyl mercury should continue to be modeled throughout Appendix B equations as individual COPCs.

TABLE B-2-5

PERVIOUS RUNOFF LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
L_R	Runoff load from pervious surfaces	g/yr	
RO	Average annual surface runoff	cm/yr	**Varies (site-specific)** This variable is site-specific. According to U.S. EPA (1993), U.S. EPA (1994), and NC DEHNR (1997), average annual surface runoff can be estimated by using the *Water Atlas of the United States* (Geraghty, Miller, Van der Leeden, and Troise 1973). According to NC DEHNR, (1997), more detailed, site-specific procedures for estimating the amount of surface runoff, such as those based on the U.S. Soil Conservation Service CNE may also be used. U.S. EPA (1985) is cited as an example of such a procedure. The following uncertainty is associated with this variable: (1) To the extent that site-specific or local average annual surface runoff information is not available, default or estimated values may not accurately represent site-specific or local conditions. As a result, K_R may be under- or overestimated to an unknown degree.
A_L	Total watershed area receiving COPC deposition	m^2	**Varies (site-specific)** This variable is site-specific (see Chapter 4). Uncertainties associated with this variable are site-specific.
A_I	Impervious watershed area receiving COPC deposition	m^2	**Varies (site-specific)** This variable is site-specific (see Chapter 4). Uncertainties associated with this variable are site-specific.
Cs	COPC concentration in soil	mg/kg	**Varies (calculated - Table B-1-1)** This value is COPC-and site-specific and should be calculated using the equation in Table B-1-1. For calculation of *Cs* in watersheds, the maximum or average of air parameter values at receptor grid nodes located within the watershed may be used (see Chapter 4). Uncertainties associated with this variable are site-specific.

TABLE B-2-5

PERVIOUS RUNOFF LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
BD	Soil bulk density	g/cm^3	**1.5** This variable is affected by the soil structure, such as looseness or compaction of the soil, depending on the water and clay content of the soil (Hillel 1980), as summarized in U.S. EPA (1990). A range of 0.83 to 1.84 was originally cited in Hoffman and Baes (1979). U.S. EPA (1994) recommended a default soil bulk density value of 1.5 g/cm^3, based on a mean value for loam soil from Carsel, Parrish, Jones, Hansen, and Lamb (1988). The value of 1.5 g/cm^3 also represents the midpoint of the "relatively narrow range" for *BD* of 1.2 to 1.7 g/cm^3. The following uncertainty is associated with this variable: (1) The recommended range of soil dry bulk density values may not accurately represent site-specific soil conditions.
θ_{sw}	Soil volumetric water content	mL/cm^3	**0.2** This variable depends on the available water and on soil structure. θ_{sw} can be estimated as the midpoint between a soil's field capacity and wilting point, if a representative watershed soil can be identified. However, U.S. EPA OSW recommends the use of 0.2 mL/cm^3 as a default value. This value is the midpoint of the range 0.1 (very sandy soils) to 0.3 (heavy loam/clay soils) recommended by U.S. EPA (1993) (no source or reference is provided for this range) and is consistent with U.S. EPA (1994). The following uncertainty is associated with this variable: (1) The default θ_{sw} values may not accurately reflect site-specific or local conditions; therefore, L_R may be under- or overestimated to a small extent, based on the limited range of values.
Kd_s	Soil-water partition coefficient	cm^3/g	**Varies (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-2. The following uncertainty is associated with this variable: (1) Uncertainties associated with this parameter will be limited if Kd_s values are calculated as described in Appendix A-2.
0.01	Units conversion factor	kg-cm^2/mg-m^2	

TABLE B-2-5

PERVIOUS RUNOFF LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

(Page 4 of 5)

REFERENCES AND DISCUSSION

Carsel, R.F., R.S. Parrish, R.L. Jones, J.L. Hansen, and R.L. Lamb. 1988. "Characterizing the Uncertainty of Pesticide Leaching in Agricultural Soils." *Journal of Contaminant Hydrology*. Volume 2: pages 11-24.

Geraghty, J.J., D.W Miller, F. Van der Leeden, and F.L. Troise. 1973. *Water Atlas of the United States*. Water Information Center. Port Washington, New York.

This document is cited by U.S. EPA (1993), U.S. EPA (1994), and NC DEHNR (1997) as a reference for calculating average annual runoff, *RO*. Specifically, this reference provides maps with isolines of annual average surface water runoff, which is defined as all flow contributions to surface water bodies, including direct runoff, shallow interflow, and ground water recharge. Because these volumes are total contributions and not only surface runoff, U.S. EPA (1994) notes that they need to be reduced to estimate surface runoff. U.S. EPA (1994) recommends a reduction of 50 percent.

Hillel, D. 1980. *Fundamentals of Soil Physics*. Academic Pres, Inc. New York.

This document is cited by U.S. EPA (1990) for the statement that dry soil bulk density, *BD*, is affected by soil structure, such as looseness or compaction of the soil, depending on the water and clay content of the soil.

Hoffman, F.O., and C.F. Baes. 1979. *A Statistical Analysis of Selected Parameters for Predicting Food Chain Transport and Internal Dose of Radionuclides*. ORNL/NUREG/TM-882.

This document presents a soil bulk density, *BD*, range of 0.83 to 1.84 g/cm^3.

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Assessments for Hazardous Waste Combustion Units*. January.

This document is one of the source documented that cites the use of the equation in Table B-2-5. However, the document is not the original source of this equation. This document also recommends the following:

- Estimation of average annual runoff, *RO* (cm/yr), by using the *Water Atlas of the United States* (Geraghty, Miller, Van der Leeden, and Troise 1973) or site-specific procedures, such as the U.S. Soil Conservation Service CNE; U.S. EPA (1985) is cited as an example of the use of the CNE
- A default value of 0.2 cm^3/cm^3 for soil volumetric content (θ_{sw})

U.S. EPA. 1985. *Water Quality Assessment: A Screening Procedures for Toxic and Conventional Pollutants in Surface and Ground Water - Part I (Revised - 1985)*. Environmental Research Laboratory. Athens, Georgia. EPA/600/6-85/002a. September.

U.S. EPA. 1990. *Interim Final Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Environmental Criteria and Assessment Office. Office of Research and Development. EPA 600-90-003. January.

This document cites Hillel (1980) for the statement that only soil bulk density, *BD*, is affected by the soil structure, such as loosened or compaction of the soil, depending on the water and clay content of the soil.

U.S. EPA. 1993. *Addendum: Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Working Group Recommendations. Office of Solid Waste and Office of Research and Development. Washington, D.C. September 24.

This document is a source of COPC-specific (inorganics only) Kd_s values used to develop a range (2 to 280,000 mL/g) of Kd_s values. This document also recommends a range of soil volumetric water content (θ_{sw}) of 0.1 cm^3/cm^3 (very sandy soils) to 0.3 cm^3/cm^3 (heavy loam/clay soils); however, no source or reference is provided for this range.

U.S. EPA. 1994. *Revised Draft Guidance of Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes*. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities. Office of Emergency and Remedial Response. Office of Solid Waste. December 14.

This document recommends (1) a default soil bulk density value of 1.5 g/cm^3, based on a mean value for loam soil from Carsel, Parrish, Jones, Hansen, and Lamb (1988), and (2) a default soil volumetric water content, θ_{sw}, value of 0.2 cm^3/cm^3, based on U.S. EPA (1993).

TABLE B-2-6

EROSION LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

Description

This equation calculates the load to the water body from soil erosion.

Uncertainties associated with this equation include the following:

(1) Most of the uncertainties associated with the variables, specifically those for X_e, A_L, A_I, and Cs, are site-specific.
(2) Uncertainties associated with the remaining variables are not expected to be significant, primarily because of the narrow ranges of probable values for these variables or the use of well-established estimation procedures (Kd_s).

Equation

$$L_E = X_e \cdot (A_L - A_I) \cdot SD \cdot ER \cdot \frac{Cs \cdot Kd_s \cdot BD}{\theta_{sw} + Kd_s \cdot BD} \cdot 0.001$$

For mercury modeling:

For mercury modeling, $L_{E\,(Initial)}$ values are calculated for divalent mercury (Hg^{2+}) and methyl mercury (MHg) using their respective Cs and Kd_s values; then as indicated below, these values are apportioned based on a 85% Hg^{2+} and 15% MHg speciation split in the water body (see Chapter 2).

$$L_{E_{Hg^{2+}}} = L_{E_{Hg^{2+}\,(Initial)}} \cdot 0.85$$

$$L_{E_{MHg}} = L_{E_{MHg\,(Initial)}} + (L_{E_{Hg^{2+}\,(Initial)}} \cdot 0.15)$$

After calculating species specific L_E values, divalent and methyl mercury should continue to be modeled throughout Appendix B equations as individual COPCs.

TABLE B-2-6

EROSION LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

(Page 2 of 6)

Variable	Description	Units	Value
L_E	Soil erosion load	g/yr	
X_e	Unit soil loss	kg/m^2-yr	**Varies (calculated - Table B-2-7)** This variable is site-specific, and is calculated by using the equation in Table B-2-7. The following uncertainty is associated with this variable: (1) All of the equation variables (see Table B-2-7) are site-specific. Use of default values rather than site-specific values, for any or all or these variables, will result in estimates of unit soil loss, X_e, that are under- or overestimated to some degree. The range of X_e calculated on the basis of default values spans slightly more than one order of magnitude (0.6 to 36.3 kg/m^2-yr).
A_L	Total watershed area receiving COPC deposition	m^2	**Varies (site-specific)** This variable is site-specific (see Chapter 4). Uncertainties associated with this variable are site-specific.
A_I	Impervious watershed area receiving COPC deposition	m^2	**Varies (site-specific)** This variable is site-specific (see Chapter 4). Uncertainties associated with this variable are site-specific.
SD	Sediment delivery ratio	unitless	**Varies (calculated - Table B-2-8)** This value is site-specific and is calculated by using the equation in Table B-2-8. The following uncertainty is associated with this variable: (1) The recommended default values for the variables *a* and *b* (empirical intercept coefficient and empirical slope coefficient, respectively) are average values, based on a review of sediment yields from various watersheds. These default values may not accurately represent site-specific watershed conditions and, therefore, may contribute to the under- or over estimation of L_E.

TABLE B-2-6

EROSION LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
ER	Soil enrichment ratio	unitless	**1 to 3** **Inorganic COPCs: 1** **Organic COPCs: 3** COPC enrichment occurs because lighter soil particles erode more than heavier soil particles and concentrations of organic COPCs which is a function of organic carbon content of sorbing media, are expected to be higher in eroded material than in-situ soil (U.S. EPA 1993). In the absence of site-specific data, U.S. EPA OSW recommends a default value of 3 for organic COPCs and 1 for inorganic COPCs. This is consistent with other U.S. EPA guidance (1993), which recommends a range of 1 to 5 and a value of 3 as a "reasonable first estimate". This range has been used for organic matter, phosphorus, and other soil-bound COPCs (U.S. EPA 1993); however, no sources or references were provided for this range. *ER* is generally higher in sandy soils than in silty or loamy soils (U.S. EPA 1993). The following uncertainty is associated with this variable: (1) The default *ER* value may not accurately reflect site-specific conditions; therefore, L_E may be over- or underestimated to an unknown, but relatively small, extent.
Cs	COPC concentration in soil	mg/kg	**Varies (calculated - Table B-1-1)** This value is COPC-and site-specific and should be calculated using the equation in Table B-1-1. For calculation of *Cs* in watersheds, the maximum or average of air parameter values at receptor grid nodes located within the watershed may be used (see Chapter 4). Uncertainties associated with this variable are site-specific.
Kd_s	Soil-water partition coefficient	cm^3/g	**Varies (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-2. The following uncertainty is associated with this variable: (1) Uncertainties associated with this parameter will be limited if Kd_s values are calculated as described in Appendix A-2.

TABLE B-2-6

EROSION LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

(Page 4 of 6)

Variable	Description	Units	Value
BD	Soil bulk density	g/cm^3	**1.5** This variable is affected by the soil structure, such as looseness or compaction of the soil, depending on the water and clay content of the soil (Hillel 1980), as summarized in U.S. EPA (1990). A range of 0.83 to 1.84 was originally cited in Hoffman and Baes (1979). U.S. EPA (1994a) recommended a default soil bulk density value of 1.5 g/cm^3, based on a mean value for loam soil from Carsel, Parrish, Jones, Hansen, and Lamb (1988). The value of 1.5 g/cm^3 also represents the midpoint of the "relatively narrow range" for *BD* of 1.2 to 1.7 g/cm^3. The following uncertainty is associated with this variable: (1) The recommended range of soil dry bulk density values may not accurately represent site-specific soil conditions.
θ_{sw}	Soil volumetric water content	mL/cm^3	**0.2** This variable depends on the available water and on soil structure. θ_{sw} can be estimated as the midpoint between a soil's field capacity and wilting point, if a representative watershed soil can be identified. However, U.S. EPA OSW recommends the use of 0.2 cm^3 as a default value. This value is the midpoint of the range of 0.1 (very sandy soils), to 0.3 (heavy loam/clay soils), recommended by U.S. EPA (1993) (no source or reference is provided for this range) and is consistent with U.S. EPA (1994). The following uncertainty is associated with this variable: (1) The default θ_{sw} values may not accurately reflect site-specific or local conditions; therefore, L_E may be under- or overestimated to a small extent, based on the limited range of values.
0.001	Units conversion factor	g/mg	

TABLE B-2-6

EROSION LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

REFERENCES AND DISCUSSION

Carsel, R.F., R.S. Parrish, R.L. Jones, J.L. Hansen, and R.L. Lamb. 1988. "Characterizing the Uncertainty of Pesticide Leaching in Agricultural Soils." *Journal of Contaminant Hydrology*. Volume 2. Pages 11-24.

This document is the source for a mean soil bulk density of 1.5 cm^3 for loam soil.

Hillel, D. 1980. *Fundamentals of Soil Physics*. Academic Press, Inc. New York.

This document is cited by U.S. EPA (1990) for the statement that dry soil bulk density, *BD*, is affected by the soil structure, such as looseness or compaction of the soil, depending on the water and clay content of the soil.

Hoffman, F.O., and C.F. Baes. 1979. *A Statistical Analysis of Selected Parameters for Predicting Food Chain Transport and Internal Dose of Radionuclides*. ORNL/NUREG/TM-882.

This document presents a soil bulk density, *BD*, range of 0.83 to 1.84 g/cm^3.

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units*. January.

This document is cited as one of the sources for the range of *BD* and Kd_s values, and the default value for the volumetric soil water content.

U.S. EPA. 1990. *Interim Final Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Environmental Criteria and Assessment Office. Office of Research and Development. EPA 600-90-003. January.

This document cites Hillel (1980) for the statement that dry soil bulk density, *BD*, is affected by the soil structure, such as looseness or compaction of the soil, depending on the water and clay content of the soil.

U.S. EPA. 1993. *Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* External Review Draft. Office of Research and Development. Washington, D.C. November 1993.

This document is the source of the recommended range of COPC enrichment ratio, *ER*, values. This range, 1 to 5, has been used for organic matter, phosphorous, and other soil-based COPCs. This document recommends a value of 3 as a "reasonable first estimate," and states that COPC enrichment occurs because lighter soil particles erode more than heavier soil particles. Lighter soil particles have higher surface-area-to-volume ratios and are higher in organic matter content. Therefore, concentrations of organic COPCs, which are a function of the organic carbon content of sorbing media, are expected to be higher in eroded material than in in-situ soil.

This document is also the source of the following:

- COPC-specific (inorganics only) Kd_s values used to develop a proposed range (0 to 280,000 mL/g) of Kd_s values

TABLE B-2-6

EROSION LOAD TO WATER BODY
(SURFACE WATER AND SEDIMENT EQUATIONS)

(Page 6 of 6)

- A range of soil volumetric water content (θ_{sw}) values of 0.1 mL/cm^3 (very gravelly soils) to 0.3 mL/cm^3 (heavy loam/clay soils); however, no source or reference is provided for this range.

U.S. EPA. 1994. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes.* Attachment C, *Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. Office of Emergency and Remedial Response. Office of Solid Waste. December 14.

This document recommends (1) a default soil bulk density value of 1.5 g/cm^3, based on a mean value for loam soil from Carsel, Parrish, Jones, Hansen, and Lamb (1988), and (2) a default soil volumetric water content, θ_{sw}, value of 0.2 cm^3, based on U.S. EPA (1993).

TABLE B-2-7

UNIVERSAL SOIL LOSS EQUATION (USLE)
(SOIL EQUATIONS)

Description

This equation calculates the soil loss rate from the watershed by using the Universal Soil Loss Equation (USLE); the result is used in the soil erosion load equation in Table B-2-6. Estimates of unit soil loss, X_e, should be determined specific to each watershed evaluated. Information on determining site- and watershed-specific values for variables used in calculating X_e is provided in U.S. Department of Agriculture (U.S. Department of Agriculture 1997) and U.S. EPA guidance (U.S. EPA 1985). Uncertainties associated with this equation include the following:

(1) All of the equation variables are site-specific. Use of site-specific values will result in estimates of unit soil loss, X_e, that are under- or overestimated to some unknown degree.

Equation

$$X_e = RF \cdot K \cdot LS \cdot C \cdot PF \cdot \frac{907.18}{4047}$$

Variable	Description	Units	Value
X_e	Unit soil loss	kg/m^2-yr	
RF	USLE rainfall (or erosivity) factor	yr^{-1}	**50 to 300 (site-specific)** This value is site-specific and is derived on a storm-by-storm basis. As cited in U.S. EPA (1993b), average annual values have been compiled regionally by Wischmeier and Smith (1978). The recommended range reflects these compiled values. The following uncertainty is associated with this variable: (1) The range of average annual rainfall factors (50 to 300) from Wischmeier and Smith (1978) may not accurately reflect site-specific conditions. Therefore, unit soil loss, X_e, may be under- or overestimated.

TABLE B-2-7

UNIVERSAL SOIL LOSS EQUATION (USLE)
(SOIL EQUATIONS)

Variable	Description	Units	Value
K	USLE erodibility factor	ton/acre	**Varies** This value is site-specific. U.S. EPA OSW recommends the use of current guidance (U.S. Department of Agriculture 1997; U.S. EPA 1985) in determining watershed-specific values for this variable based on site-specific information. A default value of 0.36, as cited in U.S. EPA (1994), was based on a soil organic matter content of 1 percent (Droppo, Strenge, Buck, Hoopes, Brockhaus, Walter, and Whelan 1989), and chosen to be representative of a whole watershed. The following uncertainty is associated with this variable: (1) The determination and use of site-specific values for the USLE soil erodibility factor, *K*, may not accurately represent site-specific conditions. Therefore, use of this value may cause unit soil loss, X_e, to be under- or overestimated.
LS	USLE length-slope factor	unitless	**Varies** This value is site-specific. U.S. EPA OSW recommends the use of current guidance (U.S. Department of Agriculture 1997; U.S. EPA 1985) in determining watershed-specific values for this variable based on site-specific information. A value of 1.5, as cited in U.S. EPA (1994), reflects a variety of possible distance and slope conditions (U.S. EPA 1988), and was chosen to be representative of a whole watershed. The following uncertainty is associated with this variable: (1) The determination and use of site-specific values for the USLE length-slope factor, *LS*, may not accurately represent site-specific conditions. Therefore, use of this value may cause unit soil loss, X_e, to be under- or overestimated.

TABLE B-2-7

UNIVERSAL SOIL LOSS EQUATION (USLE)
(SOIL EQUATIONS)

(Page 3 of 5)

Variable	Description	Units	Value
C	USLE cover management factor	unitless	**Varies** This value is site-specific. U.S. EPA OSW recommends the use of current guidance (U.S. Department of Agriculture 1997; U.S. EPA 1985) in determining watershed-specific values for this variable based on site-specific information. The range of values up to 0.1 reflect dense vegetative cover, such as pasture grass; values from 0.1 to 0.7 reflect agricultural row crops; and a value of 1.0 reflects bare soil (U.S. EPA 1993b). U.S. EPA (1993a) recommended a value of 0.1 for both grass and agricultural crops. This range of values was also cited in NC DEHNR (1997). However, U.S. EPA (1994) and NC DEHNR (1997) both recommend a default value of 0.1 to be representative of a whole watershed. The following uncertainty is associated with this variable: (1) The determination and use of site-specific values for USLE cover management factor, *C*, may not accurately represent site-specific conditions. Therefore, use of default value for *C* may result in the under- or overestimation of unit soil loss, X_e.
PF	USLE supporting practice factor	unitless	**Varies** This value is site-specific. U.S. EPA OSW recommends the use of current guidance (U.S. Department of Agriculture 1997; U.S. EPA 1985) in determining watershed-specific values for this variable based on site-specific information. A default value of 1.0, which conservatively represents the absence of any erosion or runoff control measures, was cited in U.S. EPA (1993a; 1994) and NC DEHNR (1997). The following uncertainty is associated with this variable: (1) The determination and use of site-specific values for the USLE supporting practice factor, *PF*, may not accurately represent site-specific conditions. Therefore, resulting in the under- or overestimation of unit soil loss, X_e.
907.18	Conversion factor	kg/ton	
4047	Conversion factor	m^2/acre	

TABLE B-2-7

UNIVERSAL SOIL LOSS EQUATION (USLE)
(SOIL EQUATIONS)

REFERENCES AND DISCUSSION

Droppo, J.G. Jr., D.L. Strenge, J.W. Buck, B.L. Hoopes, R.D. Brockhaus, M.B. Walter, and G. Whelan. 1989. *Multimedia Environmental Pollutant Assessment System (MEPAS) Application Guidance: Volume 2-Guidelines for Evaluating MEPAS Input Parameters*. Pacific Northwest Laboratory. Richland, Washington. December.

This document is cited by U.S. EPA 1994 and NC DEHNR 1997 as the reference source for the default USLE erodibility factor value of 0.36, based on a soil organic matter content of 1 percent.

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units*. January.

This document recommends the following:

- A USLE erodibility factor, *K*, value of 0.36 ton/acre
- A USLE length-slope factor, *LS*, value of 1.5 (unitless)
- A range of USLE cover management factor, *C*, values of 0.1 to 1; it also recommends a default value of 0.1 to be representative of a whole watershed, not just an agricultural field.
- A USLE supporting practice factor, *P*, value of 1

U.S. Department of Agriculture. 1997. *Predicting Soil Erosion by Water: A Guide to Conservation Planning With the Revised Universal Soil Loss Equation (RUSLE).* Agricultural Research Service, Agriculture Handbook Number 703. January.

U.S. EPA. 1985. *Water Quality Assessment: A Screening Procedure for Toxic and Conventional Pollutants in Surface and Ground Water—Part I (Revised).* ORD. Athens, Georgia. EPA/600/6-85/002a.

U.S. EPA. 1988. *Superfund Exposure Assessment Manual.* Office of Solid Waste. Washington, D.C. April.

This document is cited by U.S. EPA 1994 and NC DEHNR 1997 as the reference source for the USLE length-slope factor value of 1.5. This value reflects a variety of possible distance and slope conditions and was chosen to be representative of a whole watershed, not just an agricultural field.

U.S. EPA. 1993a. *Addendum: Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions. Working Group Recommendations.* Office of Solid Waste and Office of Research and Development. Washington, D.C. September 24.

This document cites Wischmeier and Smith (1978) as the source of average annual USLE rainfall factors, *RF*, and states that annual values range from less than 50 for the arid western United States to greater than 300 for the southeast.

This document also recommends the following:

- A USLE cover management factor, *C*, of 0.1 for both grass and agricultural crops
- A USLE supporting practice factor, *P*, of 1, based on the assumed absence of any erosion or runoff control measures

U.S. EPA. 1993b. *Review Draft Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustion Emissions.* Office of Health and Environmental Assessment. Office of Research and Development. EPA-600-AP-93-003. November 10.

This document discusses the USLE cover management factor. This factor, *C*, primarily reflects how erosion is influenced by vegetative cover and cropping practices, such as planting across slope rather than up and down slope. This document discusses a range of *C* values for 0.1 to 1; values greater than 0.1 but less than 0.2 are appropriate for agricultural row crops, and a value of 1 is appropriate for sites mostly devoid of vegetation.

U.S. EPA. 1994. *Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes.* Office of Emergency and Remedial Response. Office of Solid Waste. December 14.

This document recommends the following:

- A USLE erodibility factor, *K*, value of 0.36 ton/acre
- A USLE length-slope factor, *LS*, value of 1.5 (unitless)
- A range of USLE cover management factor, *C*, values of 0.1 to 1; it recommends a default value of 0.1 to be representative of a whole watershed, not just an agricultural field.
- A USLE supporting practice factor, *P*, value of 1

Wischmeire, W.H., and D.D. Smith. 1978. *Predicting Rainfall Erosion Losses—A Guide to Conservation Planning.* Agricultural Handbook No. 537. U.S. Department of Agriculture Washington, D.C.

This document is cited by U.S. EPA (1993) as the source of average annual USLE rainfall factors, *RF*, compiled regionally. According to U.S. EPA (1993), annual values range from less than 50 for the arid western United States to greater than 300 for the southeast.

TABLE B-2-8

SEDIMENT DELIVERY RATIO
(SURFACE WATER AND SEDIMENT EQUATIONS)

Description

This equation calculates the sediment delivery ratio for the watershed. The result is used in the soil erosion load equation.

Uncertainties associated with this equation include the following:

(1) The recommended default empirical intercept coefficient, *a*, values are average values based on various studies of sediment yields from various watersheds. Therefore, these default values may not accurately represent site-specific watershed conditions. As a result, use of these default values may under- or overestimate the watershed sediment delivery ratio, *SD*.

(2) The recommended default empirical slope coefficient, *b*, value is based on a review of sediment yields from various watersheds. This single default value may not accurately represent site-specific watershed conditions. As a result, use of this default value may under- or overestimate the watershed sediment delivery ratio, *SD*.

Equation

$$SD = a \cdot (A_L)^{-b}$$

Variable	Description	Units	Value
SD	Watershed sediment delivery ratio	unitless	

TABLE B-2-8

SEDIMENT DELIVERY RATIO
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
a	Empirical intercept coefficient	unitless	**0.6 to 2.1 (depends on watershed area)** This variable is site-specific and is determined on the basis of the watershed area (Vanoni 1975), as cited in U.S. EPA (1993): Watershed Area (sq. miles) / "*a*" Coefficient (unitless) ≤0.1 — 2.1 >0.1 but ≤ 1 — 1.9 >1 but ≤ 10 — 1.4 >10 but ≤ 100 — 1.2 >100 — 0.6 Note: 1 sq. mile = 2.59 x 10^6 m^2 The use of these values is consistent with U.S. EPA (1994a and 1994b) and NC DEHNR (1997). The following uncertainty is associated with this variable: (1) The recommended default empirical intercept coefficient, *a*, values are average values based on various studies of sediment yields from various watersheds. Therefore, these default values may not accurately represent site-specific watershed conditions. As a result, use of these default values may under- or overestimate the watershed sediment delivery ratio, *SD*.
A_L	Watershed area receiving COPC deposition	m^2	**Varies (site-specific)** This variable is site-specific (see Chapter 4). Uncertainties associated with this variable are site-specific.

TABLE B-2-8

SEDIMENT DELIVERY RATIO
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
b	Empirical slope coefficient	unitless	**0.125** As cited in U.S. EPA (1993), this variable is an empirical constant based on the research of Vanoni (1975), which concludes that sediment delivery ratios vary approximately with the -(1/8) power of the drainage area. The use of this value is consistent with U.S. EPA (1994a and 1994b) and NC DEHNR (1997). U.S. EPA has not completed its review of Vanoni (1975). The following uncertainty is associated with this variable: (1) The recommended default empirical slope coefficient, *b*, value is based on a review of sediment yields from various watersheds. This single default value may not accurately represent site-specific watershed conditions. As a result, use of this default value may under- or overestimate the watershed sediment delivery ratio, *SD*.

TABLE B-2-8

SEDIMENT DELIVERY RATIO
(SURFACE WATER AND SEDIMENT EQUATIONS)

(Page 4 of 4)

REFERENCES AND DISCUSSION

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units*. January.

This document is cited as one of the reference source documents for the empirical intercept coefficient, *a*, and empirical slope coefficient, *b*, values. This document cites U.S. EPA (1993) as the source of its information.

U.S. EPA. 1993. *Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* External Review Draft. Office of Research and Development. Washington, D.C. November.

This document is cited as one of the reference source documents for the empirical intercept coefficient, *a*, and empirical slope coefficient, *b*, values. This document cites Vanoni (1975) as its source of information.

U.S. EPA. 1994a. *Draft Guidance for Performing Screening Level Risk Analyses at Combustor Facilities Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. April 15.

This document is cited as one of the reference source documents for the empirical intercept coefficient, *a*, and empirical slope coefficient, *b*, values. This document does not identify Vanoni (1975) as the source of its information.

U.S. EPA. 1994b. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. Office of Emergency and Remedial Response. Office of Solid Waste. December 14.

This document is cited as one of the reference source documents for the empirical intercept coefficient, *a*, and the empirical slope coefficient, *b*, values. This document cites U.S. EPA (1993) as the source of its information.

Vanoni, V.A. 1975. *Sedimentation Engineering*. American Society of Civil Engineers. New York, New York. Pages 460-463.

This document is cited by U.S. EPA (1993) as the source of the equation in Table B-2-8 and the empirical intercept coefficient, *a*, and empirical slope coefficient, *b*, values. Based on various studies of sediment yields from watersheds, this document concludes that the sediment delivery ratios vary approximately with the -(1/8) power of the drainage ratio.

TABLE B-2-9

TOTAL WATER BODY CONCENTRATION
(SURFACE WATER AND SEDIMENT EQUATIONS)

Description

This equation calculates the total water body concentration; including the water column and the bed sediment.

Uncertainties associated with this equation include the following:

(1) The default variable values recommended for use in the equation in Table B-2-9 may not accurately represent site-specific water body conditions. The degree of uncertainty associated with the variables Vf_x, A_W, d_{wc}, *and* d_{bs} is expected to be limited either because the probable ranges for these variables are narrow or information allowing accurate estimates is generally available.

(2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default organic carbon (*OC*) content values and may be significant in specific instances. Uncertainties associated with the total core load into water body (L_T) and overall total water body core dissipation rate constant (k_{wt}) may also be significant in some instances because of the summation of many variable-specific uncertainties.

Equation

$$C_{wtot} = \frac{L_T}{Vf_x \cdot f_{wc} + k_{wt} \cdot A_W \cdot \left(d_{wc} + d_{bs}\right)}$$

For mercury modeling:

Total water body concentration is calculated for divalent mercury (Hg^{2+}) and methyl mercury (MHg) using their respective L_T values, f_{wc} values, and k_{wt} values.

Variable	Description	Units	Value
C_{wtot}	Total water body COPC concentration (including water column and bed sediment)	g/m^3 (equivalent to mg/L)	
L_T	Total COPC load to the water body (including deposition, runoff, and erosion)	g/yr	**Varies (calculated - Table B-2-1)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-1. Uncertainties associated with L_{DEP}, L_{Dif}, L_{RI}, L_R, *and* L_E, as presented in Table B-2-1, are also associated with L_T.

TABLE B-2-9

TOTAL WATER BODY CONCENTRATION (SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
Vf_x	Average volumetric flow rate through water body	m^3/yr	**Varies (site-specific)** This variable is site-specific and should be an annual average. The following uncertainty is associated with this variable: (1) Use of default average volumetric flow rate (Vf_x) information may not accurately represent site-specific conditions, especially for those water bodies for which flow rate information is not readily available. Therefore, use of default Vf_x values may contribute to the under- or overestimation of total water body COPC concentration, C_{wtot}.
f_{wc}	Fraction of total water body COPC concentration that occurs in the water column	unitless	**0 to 1 (calculated - Table B-2-10)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-10. The following uncertainty is associated with this variable: (1) The default values for the variables in the equation in Table B-2-10 may not accurately represent site- and water body - specific conditions. However, the range of several variables—including d_{bs}, C_{BS}, *and* θ_{bs}—is relatively narrow. Other variables, such as d_{wc} and d_z, can be reasonably estimated on the basis of generally available information. The largest degree of uncertainty may be introduced by the default medium-specific organic carbon (*OC*) content values. Because *OC* content values may vary widely in different locations in the same medium, by using default values may result in insignificant uncertainty in specific cases.
k_{wt}	Overall total water body COPC dissipation rate constant	yr^{-1}	**Varies (calculated - Table B-2-11)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-11. The following uncertainty is associated with this variable: (1) All of the variables in the equation in Table B-2-11 are site-specific; therefore, the use of default values for any or all of these variables will contribute to the under- or overestimation of C_{wtot}. The degree of uncertainty associated with the variable k_b is expected to be under one order of magnitude and is associated largely with the estimation of the unit soil loss, X_e, values for the variables f_{wc}, k_v, and f_{bs} are dependent on medium-specific estimates of *OC* content. Because *OC* content can vary widely for different locations in the same medium, uncertainty associated with these three may be significant in specific instances.

TABLE B-2-9

TOTAL WATER BODY CONCENTRATION
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
A_W	Water body surface area	m^2 (average value for the entire year)	**Varies (site-specific)** This variable is site-specific (see Chapter 4). The value selected is assumed to represent an average value for the entire year. Uncertainties associated with this variable are site-specific and expected to be limited, because maps, aerial photographs, and other resources from which water body surface areas can be measured, are readily available.
d_{wc}	Depth of water column	m (average value for the entire year)	**Varies (site-specific)** This variable is site-specific and should be an average annual value. The following uncertainty is associated with this variable: (1) Use of default depth of water column, d_{wc}, values may not accurately reflect site-specific conditions, especially for those water bodies for which depth of water column information is unavailable or outdated. Therefore, use of default d_{wc} values may contribute to the under-or overestimation of total water body COPC concentration, C_{wtot}.
d_{bs}	Depth of upper benthic sediment layer	m	**0.03** This variable is site-specific. The value selected is assumed to represent an average value for the entire year. U.S. EPA OSW recommends a default upper benthic sediment depth of 0.03 meter, which is consistent with U.S. EPA (1994) and NC DEHNR (1997) guidance. This range was cited by U.S. EPA (1993); however, no reference was cited for this range. The following uncertainty is associated with this variable: (1) Use of default depth of upper benthic layer, d_{bs}, values may not accurately represent site-specific water body conditions. However, based on the narrow recommended range, any uncertainty introduced is expected to be limited.

TABLE B-2-9

TOTAL WATER BODY CONCENTRATION
(SURFACE WATER AND SEDIMENT EQUATIONS)

REFERENCES AND DISCUSSION

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units.* January.

This document is also cited as one of the reference source documents for the default depth of upper benthic layer value. The default value is the midpoint of an acceptable range. This document cites U.S. EPA (1993) as its source of information for the range of values for the depth of the upper benthic layer.

U.S. EPA. 1993. *Addendum: Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Working Group Recommendations. Office of Solid Waste and Office of Research and Development. Washington, D.C. September 24.

This document is cited by NC DEHNR (1997) and U.S. EPA (1994) as the source of the range and default value for the depth of the upper benthic layer (d_{bs}).

U.S. EPA. 1994. *Draft Guidance for Performing Screening Level Risk Analyses at Combustor Facilities Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. April 15.

This document is cited as one of the reference source documents for the default depth of the upper benthic layer value. The default value is the midpoint of an acceptable range. This document cites U.S. EPA (1993) as its source of information for the range of values for the depth of the upper benthic layer.

TABLE B-2-10

FRACTION IN WATER COLUMN AND BENTHIC SEDIMENT (SURFACE WATER AND SEDIMENT EQUATIONS)

Description

This equation calculates the fraction of total water body concentration occurring in the water column and the bed sediments.

Uncertainties associated with this equation include the following:

(1) The default variable values may not accurately represent site-specific water body conditions. However, the range of several variables—including d_{bs}, BS, and θ_{bs}—is relatively narrow. Other variables, such as d_{wc} and d_z, can be reasonably estimated on the basis of generally available information. The largest degree of uncertainty may be introduced by the default medium-specific OC content values. OC content values can vary widely for different locations in the same medium. Therefore, the use of default values may introduce significant uncertainty in some cases.

Equations

$$f_{wc} = \frac{(1 + Kd_{sw} \cdot TSS \cdot 10^{-6}) \cdot d_{wc}/d_z}{(1 + Kd_{sw} \cdot TSS \cdot 1x10^{-6}) \cdot d_{wc}/d_z + (\theta_{bs} + Kd_{bs} \cdot BS) \cdot d_{bs}/d_z}$$

$$f_{bs} = 1 - f_{wc}$$

For mercury modeling:

The fraction in water column (f_{wc}) is calculated for divalent mercury (Hg^{2+}) and methyl mercury (MHg) using their respective Kd_{sw} values and Kd_{bs} values.
The fraction in benthic sediment (f_{bs}) is calculated for divalent mercury (Hg^{2+}) and methyl mercury (MHg) using their respective f_{wc} values.

Variable	Description	Units	Value
f_{wc}	Fraction of total water body COPC concentration in the water column	unitless	
f_{bs}	Fraction of total water body COPC concentration in the benthic sediment	unitless	

TABLE B-2-10

FRACTION IN WATER COLUMN AND BENTHIC SEDIMENT (SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
Kd_{sw}	Suspended sediments/surface water partition coefficient	L/kg	**Varies (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-2. The following uncertainty is associated with this variable: (1) The Kd_{sw} values in Appendix A-2 are based on default *OC* contents for surface water and soil. Kd_{sw} values based on default values may not accurately reflect site- and water body-specific conditions and may under- or overestimate actual Kd_{sw} values. Uncertainty associated with this variable will be reduced if site-specific and medium-specific *OC* estimates are used to calculate Kd_{sw}.
TSS	Total suspended solids concentration	mg/L	**2 to 300** This variable is site-specific. U.S. EPA OSW recommends the use of site- and waterbody specific measured values, representative of long-term average annual values for the water body of concern (see Chapter 3). A value of 10 mg/L was cited by NC DEHNR (1997), U.S. EPA (1993a), and U.S. EPA (1993b) in the absense of site-specific measured data. The following uncertainty is associated with this variable: Limitation on measured data used for determining a water body specific total suspended solids (*TSS*) value may not accurately reflect site- and water body-specific conditions long term. Therefore, the *TSS* value may contribute to the under-or overestimation of f_{wc}.
10^{-6}	Units conversion factor	kg/mg	
d_{wc}	Depth of water column	m	**Varies (site-specific)** This variable is site-specific and should be an average annual value. The following uncertainty is associated with this variable: (1) Use of default depth of water column, d_{wc}, values may not accurately reflect site-specific conditions, especially for those water bodies for which depth of water column information is unavailable or outdated. Therefore, use of default d_{wc} values may contribute to the under- or overestimation of total water body COPC concentration, C_{wtot}.

TABLE B-2-10

FRACTION IN WATER COLUMN AND BENTHIC SEDIMENT (SURFACE WATER AND SEDIMENT EQUATIONS)

(Page 3 of 5)

Variable	Description	Units	Value
d_{bs}	Depth of upper benthic sediment layer	m	**0.03** This variable is site-specific. U.S. EPA OSW recommends a default upper benthic sediment depth of 0.03 meter, which is consistent with U.S. EPA (1994) and NC DEHNR (1997) guidance. This range was cited by U.S. EPA (1993b); however, no reference was cited for this range. The following uncertainty is associated with this variable: (1) Use of default depth of upper benthic layer, d_{bs}, values may not accurately represent site-specific water body conditions. However, any uncertainly introduced is expected to be limited on the basis of the narrow recommended range.
d_z	Total water body depth	m	**Varies (calculated)** This variable is site-specific. U.S. EPA OSW recommends that the following equation be used to calculate total water body depth, consistent with NC DEHNR (1997): $d_z = d_{wc} + d_{bs}$ The following uncertainty is associated with this variable: (1) Calculation of this variable combines the concentrations associated with the two variables (d_{wc} and d_{bs}) being summed. Because most of the total water body depth (d_z) is made up of the depth of the water column (d_{wc}), and the uncertainties associated with d_{wc} are not expected to be significant, the total uncertainties associated with this variable, d_z, are also not expected to be significant.
BS	Benthic solids concentration	g/cm^3 (equivalent to kg/L)	**1.0** This variable is site-specific. U.S. EPA OSW recommends a default value of 1.0, consistent with U.S. EPA (1993a), which states that this value should be reasonable for most applications. The recommended default value is also consistent with other U.S. EPA (1993b and 1994) and NC DEHNR (1997) guidance. The following uncertainty is associated with this variable: (1) The recommended default value may not accurately represent site- and water body-specific conditions. Therefore, the variable f_{wc} may be under- or overestimated; the assumption that the under- or overestimation will be limited is based on the narrow recommended range.

TABLE B-2-10

FRACTION IN WATER COLUMN AND BENTHIC SEDIMENT (SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
θ_{bs}	Bed sediment porosity	$L_{water}/L_{sediment}$	**0.6** This variable is site-specific. U.S. EPA OSW recommends a default bed sediment porosity of 0.6 (by using a *BS* value of 1 g/cm^3 and a solid density (ρ_s) value of 2.65 kg/L, calculated by using the following equation (U.S. EPA 1993a): $\theta_{bs} = 1 - BS/\rho_s$ This is consistent with other U.S. EPA (1993b and 1994) guidance. The following uncertainty is associated with this variable: (1) Calculation of this variable combines the uncertainties associated with the two variables (*BS* and ρ_s) used in the calculation. To the extent that the recommended default values of *BS* and ρ_s do not accurately represent site- and water body-specific conditions, θ_{bs} will be under- or overestimated.
Kd_{bs}	Bed sediment/sediment pore water partition coefficient	L/kg	**Varies (see Appendix A-2)** This variable is COPC-specific, and should be determined from the COPC tables in Appendix A-2. The following uncertainty is associated with this variable: (1) The Kd_{bs} values in Appendix A-2 are based on default *OC* contents for sediment and soil. Kd_{bs} values based on default *OC* values may not accurately represent site- and water body-specific conditions and may under- or overestimate actual Kd_{bs} values. Uncertainty associated with this variable will be reduced if site- and water body-specific *OC* estimates are used to calculate Kd_{bs}.

TABLE B-2-10

FRACTION IN WATER COLUMN AND BENTHIC SEDIMENT (SURFACE WATER AND SEDIMENT EQUATIONS)

REFERENCES AND DISCUSSION

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units.* January.

This document is cited as one of the sources of the range of Kd_s values and assumed *OC* values of 0.075 and 0.04 for surface water and sediment, respectively. This document is also cited as one of the sources of TSS. This document cites U.S. EPA (1993b) as its source of information. This document is also cited as the source of the equation for calculating total water body depth. No source of this equation was identified. This document is also cited as one of the reference source documents for the default value for bed sediment porosity. This document cites U.S. EPA (1993b) as its source of information. This document is also cited as one of the reference source documents for the default value for depth of the upper benthic layer. The default value is the midpoint of an acceptable range. This document cites U.S. EPA (1993b) as its source of information for the range of values for the depth of the upper benthic layer. This document is also cited as one of the reference source documents for the default bed sediment concentration.

U.S. EPA. 1993a. *Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* External Review Draft. Office of Research and Development. Washington, D.C. November 1993.

This document is cited as one of the sources of the range of Kd_s values and assumed *OC* values of 0.075 and 0.04 for surface water and sediment, respectively. The generic equation for calculating partition coefficients (soil, surface water, and bed sediments) is as follows: $Kd_{ij} = Koc * OC_i$. *Koc* is a chemical-specific value; however, *OC* is medium-specific. The range of Kd_s values was based on an assumed *OC* value of 0.01 for soil. Kd_{sw} and Kd_{bs} values were estimated by multiplying the Kd_s values by 7.5 and 4, because the *OC* values for surface water and sediment are 7.5 and 4 times greater than the *OC* value for soil. This document also presents the equation for calculating bed sediment porosity (θ_{bs}); no source of this equation was identified. This document was also cited as the source for the range of the benthic solids concentration (BS); no original source of this range was identified. Finally, this document recommends that, in the absence of site-specific information, a *TSS* value of 1 to 10 be specified for parks and lakes, and a *TSS* value of 10 to 20 be specified in streams and rivers.

U.S. EPA. 1993b. *Addendum: Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Working Group Recommendations. Office of Solid Waste and Office of Research and Development. Washington, D.C. September 24.

This document is cited by NC DEHNR (1997) as the source of the *TTS* value. This document is also cited by NC DEHNR (1997) and U.S. EPA (1994) as the source of the default bed sediment porosity value and the equation used to calculate the variable, the default bed sediment concentration value, and the range for the depth of the upper benthic layer values.

U.S. EPA. 1994. *Draft Guidance for Performing Screening Level Risk Analyses at Combustor Facilities Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. April 15.

This document is cited as one of the reference source documents for the default value for bed sediment porosity. This document cites U.S. EPA (1993b) as its source of information. This document is also cited as one of the reference source documents for the default value for depth of the upper benthic layer. The default value is the midpoint of an acceptable range. This document cites U.S. EPA (1993b) as its source of information for the range of values for the depth of the upper benthic layer. This document is also cited as one of the reference source documents for the default benthic solids concentration.

TABLE B-2-11

OVERALL TOTAL WATER BODY DISSIPATION RATE CONSTANT (SURFACE WATER AND SEDIMENT EQUATIONS)

Description

This equation calculates the overall dissipation rate of COPCs in surface water, resulting from volatilization and benthic burial.

Uncertainties associated with this equation include the following:

(1) All of the variables in the equation in Table B-2-11 are site-specific. Therefore, the use of default values for any or all of these variables will contribute to the under- or overestimation of k_{wt}. The degree of uncertainty associated with the variable k_b is expected to be one order of magnitude at most and is associated with the estimation of the unit soil loss, X_e. Values for the variables f_{wc}, k_v, and f_{bs} are dependent on medium-specific estimates of medium-specific *OC* content. Because *OC* content can vary widely for different locations in the same medium, uncertainty associated with these three variables may be significant in specific instances.

Equation

$$k_{wt} = f_{wc} \cdot k_v + f_{bs} \cdot k_b$$

Variable	Description	Units	Value
k_{wt}	Overall total water body dissipation rate constant	yr^{-1}	
f_{wc}	Fraction of total water body COPC concentration in the water column	unitless	**Varies (calculated - Table B-2-10)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-10. Uncertainties associated with this variable include the following: (1) The default variable values recommended for use in the equation in Table B-2-10 may not accurately represent site-specific water body conditions. However, the range of several variables—including d_{bs}, *BS*, and θ_{sw}—is moderate (factors of 5, 3, and 2, respectively); therefore, the degree of uncertainty associated with these variables is expected to be moderate. Other variables, such as d_{wc} and d_z, can be reasonably estimated on the basis of generally available information; therefore, the degree of uncertainty associated with these variables is expected to be relatively small. (2) The largest degree of uncertainty may be introduced by the default medium-specific *OC* content values. *OC* content values are often not readily available and can vary widely for different locations in the same medium. Therefore, the degree of uncertainty may be significant in specific instances.

TABLE B-2-11

OVERALL TOTAL WATER BODY DISSIPATION RATE CONSTANT (SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
k_v	Water column volatilization rate constant	yr^{-1}	**Varies (calculated - Table B-2-13)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-13. Uncertainties associated with this variable include the following: (1) All of the variables in Table B-2-13 are site-specific. Therefore, the use of default values for any or all of these variables could contribute to the under- or overestimation of k_v. (2) The degree of uncertainty associated with the variables d_z and *TSS* is expected to be minimal either because information necessary to estimate these variables is generally available or because the range of probable values is narrow. (3) Values for the variable k_v and Kd_{sw} are dependent on medium-specific estimates of *OC* content. Because *OC* content can vary widely for different locations in the same medium, uncertainty associated with these two variables may be significant in specific instances.
f_{bs}	Fraction of total water body COPC concentration in the benthic sediment	unitless	**Varies (calculated - Table B-2-10)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-10. Uncertainties associated with this variable include the following: (1) The default variable values recommended for use in the equation in Table B-2-10 may not accurately represent site-specific water body conditions. However, the range of several variables—including d_{bs}, *BS*, and θ_{sw}—is relatively narrow; therefore, the degree of uncertainty associated with these variables is expected to be relatively small. Other variables, such as d_{wc} and d_z, can be reasonably estimated on the basis of generally available information. (2) The largest degree of uncertainty may be introduced by the default medium-specific *OC* contact values. *OC* content values are often not readily available and can vary widely for different locations in the same medium. Therefore, the degree of uncertainty may be significant in specific instances.
k_b	Benthic burial rate constant	yr^{-1}	**Varies (calculated - Table B-2-16)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-16. Uncertainties associated with this variable include the following: (1) All of the variables in Table B-2-16 are site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of k_b. (2) The degree of uncertainty associated with each of these variables is as follows: (1) X_e—about one order of magnitude at most, (2) *BS* , d_{bs}, Vf_x, *TSS*, and A_w—limited because of the narrow recommended ranges for these variables or because resources to estimate variable values are generally available, and (3) A_L and *SD*—very site-specific and degree of uncertainty unknown.

TABLE B-2-12

WATER COLUMN VOLATILIZATION LOSS RATE CONSTANT
(SURFACE WATER AND SEDIMENT EQUATIONS)

Description

This equation calculates the water column of COPCs loss resulting from volatilization. Uncertainties associated with this equation include the following:

(1) All of the variables in Table B-2-12 are site-specific. Therefore, the use of default values for any or all of these variables will contribute to the under- or over estimation of k_v. The degree of uncertainty associated with the variables d_{wc}, d_{bs}, d_z, and *TSS* are expected to be minimal either because information necessary to estimate these variables is generally available or because the range of probable values is narrow. Values for the variables K_v and Kd_{sw} are dependent on medium-specific estimates of *OC* content. Because *OC* content can vary widely for different locations in the same medium, uncertainty associated with these two variables may be significant in specific instances.

Equation

$$k_v = \frac{K_v}{d_z \cdot (1 + Kd_{sw} \cdot TSS \cdot 10^{-6})}$$

For mercury modeling:

The water column volatilization loss rate constant is calculated for divalent mercury (Hg^{2+}) and methyl mercury (MHg) using their respective fate and transport parameters .

Variable	Description	Units	Value
k_v	Water column volatilization rate constant	yr^{-1}	

TABLE B-2-12

WATER COLUMN VOLATILIZATION LOSS RATE CONSTANT (SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
K_v	Overall COPC transfer rate coefficient	m/yr	**Varies (calculated - Table B-2-13)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-13. Uncertainties associated with this variable include the following: (1) All of the variables in Table B-2-13—except *R*, the universal gas constant, which is well-established—are site-specific. Therefore, the use of default values, for any or all these variables, could contribute to the under- or overestimation of K_v. (2) The degree of uncertainty associated with the variables *H* and T_{wk} is expected to be minimal; values for *H* are well-established, and average water body temperature, T_{wk}, will likely vary less than 10 percent of the default value. (3) The uncertainty associated with the variables K_L and K_G is attributable largely to medium-specific estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, the use of default values may generate significant uncertainty in specific instances. Finally, the origin of the recommended θ value is unknown; therefore, the degree of associated uncertainty is also unknown.
d_{wc}	Depth of water column	m	**Varies (site-specific)** This variable is site-specific and should be an average annual value. The following uncertainty is associated with this variable: (1) Use of default values for depth of water column, d_{wc}, may not accurately reflect site-specific conditions, especially for those water bodies for which depth of water column information is unavailable or outdated. Therefore, use of default d_{wc} values may contribute to the under- or overestimation of total water body COPC concentration, C_{wtot}. However, the degree of under- or overestimation is not expected to be significant.
d_{bs}	Depth of upper benthic sediment layer	m	**0.03** This variable is site-specific. U.S. EPA OSW recommends a default upper-benthic sediment depth of 0.03 meter, which is based on the center of this range cited by U.S. EPA (1993b). This is consistent with U.S. EPA (1994) and NC DEHNR (1997). The following uncertainty is associated with this variable: (1) Use of default values for depth of upper benthic layer, d_{bs}, may not accurately represent site-specific water body conditions. However, any uncertainty introduced is expected to be limited, based on the narrow recommended range.

TABLE B-2-12

WATER COLUMN VOLATILIZATION LOSS RATE CONSTANT
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
d_z	Total water body depth	m	**Varies (calculated)** This variable is site-specific. U.S. EPA OSW recommends that the following equation be used to calculate total water body depth, consistent with NC DEHNR (1997): $d_z = d_{wc} + d_{bs}$ The following uncertainty is associated with this variable: (1) Calculation of this variable combines the concentrations associated with the two variables (d_{wc} and d_{bs}) being summed. Because most of the total water body depth (d_z) is made up of the depth of the water column (d_{wc}), and the uncertainties associated with d_{wc} are not expected to be significant, the total uncertainties associated with this variable, d_z, are also not expected to be significant.
Kd_{sw}	Suspended sediments/surface water partition coefficient	L/kg	**Varies (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-3. The following uncertainty is associated with this variable: (1) The values contained in Appendix A-2 for Kd_{sw} are calculated on the basis of default *OC* contents for surface water and soil. Kd_{sw} values based on default values may not accurately reflect site-and water body-specific conditions and may under- or overestimate actual Kd_{sw} values. Uncertainty associated with this variable will be reduced if site-specific and medium-specific *OC* estimates are used to calculate Kd_{sw}.
TSS	Total suspended solids concentration	mg/L	**2 to 300** This variable is site-specific. U.S. EPA OSW recommends the use of site- and waterbody specific measured values, representative of long-term average annual values for the water body of concern (see Chapter 3). A value of 10 mg/L was cited by NC DEHNR (1997), U.S. EPA (1993a), and U.S. EPA (1993b) in the absense of site-specific measured data. The following uncertainty is associated with this variable: Limitation on measured data used for determining a water body specific total suspended solids (*TSS*) value may not accurately reflect site- and water body-specific conditions long term. Therefore, the *TSS* value may contribute to the under-or overestimation of f_{wc}.
10^{-6}	Units conversion factor	kg/mg	

TABLE B-2-12

WATER COLUMN VOLATILIZATION LOSS RATE CONSTANT (SURFACE WATER AND SEDIMENT EQUATIONS)

REFERENCES AND DISCUSSION

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units.* January.

This document is cited as the source of the equation for calculating total water body depth. No source of this equation was identified. This document is also cited as one of the sources of the range of Kd_s values and an assumed *OC* value of 0.075 for surface water. This document is also cited as one of the sources of *TSS.* This document cites U.S. EPA (1993b) as its source of information.

U.S. EPA. 1993a. *Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* External Review Draft. Office of Research and Development. Washington, D.C. November 1993.

This document is cited as one of the sources of the range of Kd_s values and assumed *OC* content value of 0.075 for surface water. The generic equation for calculating partition coefficients (soil, surface water, and bed sediments) is as follows: $Kd_{ij} = K_{ocj}\ OC_i$. K_{oc} is a chemical-specific value; however, *OC* is medium-specific. The range of Kd_s values was based on an assumed *OC* value of 0.01 for soil. This document is one of the sources cited that assumes an *OC* value of 0.075 for surface water. Therefore, the Kd_{sw} value was estimated by multiplying the Kd_s values by 7.5, because the *OC* value for surface water is 7.5 times greater than the *OC* value for soil.

U.S. EPA. 1993b. *Addendum: Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Working Group Recommendations. Office of Solid Waste and Office of Research and Development. Washington, D.C. September 24.

This document is cited by U.S. EPA (1994) and NC DEHNR (1997) as the source of the range and default value for the depth of the upper benthic layer (d_{bs}). This document is also cited by NC DEHNR (1997) as the source of the *TSS* value.

U.S. EPA. 1994. *Draft Guidance for Performing Screening Level Risk Analysis at Combustion Facility Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facility*. April 15.

This document is cited as one of the reference source documents for the default value of the depth of the upper benthic layer. The default value is the midpoint of an acceptable range. This document cites U.S. EPA (1993b) as its source of information.

TABLE B-2-13

OVERALL COPC TRANSFER RATE COEFFICIENT (SURFACE WATER AND SEDIMENT EQUATIONS)

Description

This equation calculates the overall transfer rate of contaminants from the liquid and gas phases in surface water.

Uncertainties associated with this equation include the following:

(1) All of the variables in Table B-2-13—except *R*, the universal gas constant, which is well-established—are site-specific. Therefore, the use of any or all of these variables will contribute to the under- or overestimation of K_v. The degree of uncertainty associated with the variables *H* and T_{wk} is expected to be minimal; values for *H* are well-established, and average water body temperature will likely vary less than 10 percent of the default value. The uncertainty associated with the variables K_v and K_G is attributable largely to medium-specific estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, the use of default values may generate significant uncertainty in specific instances.

Equation

$$K_v = \left[K_L^{-1} + \left(K_G \cdot \frac{H}{R \cdot T_{wk}} \right)^{-1} \right]^{-1} \cdot \theta^{(T_{wk} - 293)}$$

For mercury modeling:

The overall COPC transfer rate coefficient is calculated for divalent mercury (Hg^{2+}) and methyl mercury (MHg) using their respective fate and transport parameters.

Variable	Description	Units	Value
K_v	Overall COPC transfer rate coefficient	m/yr	

TABLE B-2-13

OVERALL COPC TRANSFER RATE COEFFICIENT
(SURFACE WATER AND SEDIMENT EQUATIONS)

Page (2 of 4)

Variable	Description	Units	Value
K_L	Liquid-phase transfer coefficient	m/yr	**Varies (calculated - Table B-2-14)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-14. Uncertainties associated with this variable include the following: All of the variables in Table B-2-14 are site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of K_v. The degree of uncertainty associated with these variables is as follows: (1) Minimal or insignificant uncertainty is assumed to be associated with six variables—D_w, u, d_z, ρ_a, ρ_w, and μ_w—either because of narrow recommended ranges for these variables or because information to estimate variable values is generally available. (2) No original sources were identified for the equations used to derive recommended values or specific recommended values for variables Cd, k, and λ_z. Therefore, the degree and direction of any uncertainties associated with these variables are unknown. (3) Uncertainties associated with the variable W are site-specific.
K_G	Gas-phase transfer coefficient	m/yr	**Varies (calculated - Table B-2-15)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-15. Uncertainties associated with this variable include the following: All of the variables in Table B-2-15, with the exception of k, are site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of K_G. The degree of uncertainty associated with each of these variables is as follows: (1) Minimal or insignificant uncertainty is assumed to be associated with the variables D_a, μ_a, and ρ_a, because these variables have been extensively studied, and equation procedures are well-established. (2) No original sources were identified for equations used to derive recommended values or specific recommended values for variables C_d, k, and d_z. Therefore, the degree and direction of any uncertainties are unknown. (3) Uncertainties associated with the variable W are site-specific and cannot be readily estimated.

TABLE B-2-13

OVERALL COPC TRANSFER RATE COEFFICIENT
(SURFACE WATER AND SEDIMENT EQUATIONS)

Page (3 of 4)

Variable	Description	Units	Value
H	Henry's Law constant	atm-m^3/mol	**Varies (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-2. The following uncertainty is associated with this variable: (1) Values for this variable, estimated by using the parameters and algorithms in Appendix A-2, may under- or overestimate the actual COPC-specific values. As a result, K_v may be under- or overestimated to a limited degree.
R	Universal gas constant	atm-m^3/mol-K	**8.205 x 10^{-5}** There are no uncertainties associated with this parameter.
T_{wk}	Water body temperature	K	**298** This variable is site-specific. U.S. EPA OSW recommends the use of this default value when site-specific information is not available; this is consistent with U.S. EPA (1993a; 1993b; and 1994). The following uncertainty is associated with this variable: (1) To the extent that the default Water body temperature value does not accurately represent site- and water body-specific conditions, K_v, will be under- or overestimated to a limited degree.
θ	Temperature correction factor	unitless	**1.026** This variable is site-specific. U.S. EPA OSW recommends the use of this default value when site-specific information is not available; this is consistent with U.S. EPA (1993a; 1993b; and 1994). The following uncertainty is associated with this variable: (1) The purpose and sources of this variable and the recommended value are unknown.

TABLE B-2-13

OVERALL COPC TRANSFER RATE COEFFICIENT (SURFACE WATER AND SEDIMENT EQUATIONS)

REFERENCES AND DISCUSSION

U.S. EPA. 1993a. *Addendum: Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. Working Group Recommendations. Office of Solid Waste and Office of Research and Development. Washington, D.C. September 24.

This document is the reference source for the equation in Table B-2-12, including the use of the temperature correction fraction (θ).

This document is also cited by U.S. EPA (1994) as the source of the T_{wk} value of 298 K (298 K = 25°C) and the default θ value of 1.026.

U.S. EPA. 1993b *Addendum to Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* External Review Draft. Office of Solid Waste and Office Research and Development. Washington, D.C. November 10.

This document recommends the T_{wk} value of 298 K (298 K = 25 °C) and the value θ of 1.026. No source was identified for these values.

U.S. EPA 1994. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes*. *Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. Office of Emergency and Remedial Response. Office of Solid Waste. December 14.

This document is cited as the reference source for water body temperature (T_{wk}) and temperature correction factor (θ). This document apparently cites U.S. EPA (1993a) as its source of information.

TABLE B-2-14

LIQUID-PHASE TRANSFER COEFFICIENT
(SURFACE WATER AND SEDIMENT EQUATIONS)

Description

This equation calculates the rate of contaminant transfer from the liquid phase for a flowing or quiescent system.

Uncertainties associated with this equation include the following:

(1) Minimal or insignificant uncertainly is assumed to be associated with the following six variables: D_w, d_z, ρ_a, ρ_w, *and* μ_w.
(2) No original sources were identified for equations used to derive recommended values or specific recommended values for the following three variables: C_d, k, and d_z. Therefore, the degree and duration of any uncertainties associated with these variables is unknown.
(3) Uncertainties associated with the variable W are site-specific.

Equation

For flowing streams or rivers

$$K_L = \sqrt{\frac{10^{-4} \cdot D_w \cdot u}{d_z}} \cdot 3.1536 \times 10^7$$

For quiescent lakes or ponds

$$K_L = (C_d^{0.5} \cdot W) \cdot \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \cdot \left(\frac{k^{0.33}}{\lambda_z}\right) \cdot \left(\frac{\mu_w}{\rho_w \cdot D_w}\right)^{-0.67} \cdot 3.1536 \times 10^7$$

For mercury modeling:

The liquid phase transfer coefficient is calculated for divalent mercury (Hg^{2+}) and methyl mercury (MHg) using their respective fate and transport parameters .

TABLE B-2-14

LIQUID-PHASE TRANSFER COEFFICIENT
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
K_L	Liquid-phase transfer coefficient	m/yr	
D_w	Diffusivity of COPC in water	cm^2/s	**Varies (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC physical and chemical parameter tables in Appendix A-2. The following uncertainty is associated with this variable: (1) The default D_w values may not accurately represent the behavior of COPCs under water body-specific conditions. However, the degree of uncertainty is expected to be minimal.
u	Current velocity	m/s	**Varies (site-specific)** This variable is site-specific. The following uncertainty is associated with this variable: (1) Sources of values for this variable are reasonably available for most large surface water bodies. Estimated values for this variable be necessary for smaller water bodies; uncertainty will be associated with these estimates. The degree of uncertainty associated with this variable is not expected to be significant.

TABLE B-2-14

LIQUID-PHASE TRANSFER COEFFICIENT (SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
d_z	Total water body depth	m	**Varies (calculated)** This variable is site-specific. U.S. EPA OSW recommends that this value be calculated by using the following equation, consistent with U.S. EPA (1994): $d_z = d_{wc} + d_{bs}$ No reference was cited for this recommendation. The following uncertainty is associated with this variable: (1) Calculation of this variable combines the concentrations associated with the two variables (d_{wc} and d_{bs}) being summed. Because most of the total water body depth (d_z) is made up of the depth of the water column (d_{wc}), and the uncertainties associated with d_{wc} are not expected to be significant, the total uncertainties associated with this variable, d_z, are also not expected to be significant.
3.1536×10^7	Units conversion constant	s/yr	
C_d	Drag coefficient	unitless	**0.0011** This variable is site-specific. U.S. EPA OSW recommends a default value of 0.0011, consistent with U.S. EPA (1993a; 1993b; 1994) and NC DEHNR (1997). The following uncertainty is associated with this variable: (1) The original source of this variable value is unknown. Therefore, any uncertainties associated with its use are also unknown.
W	Average annual wind speed	m/s	**3.9** Consistent with U.S. EPA (1990), U.S. EPA OSW recommends a default value of 3.9 m/s. See Chapter 3 for guidance regarding the references and methods used to determine site-specific values for air dispersion modeling.

TABLE B-2-14

LIQUID-PHASE TRANSFER COEFFICIENT
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
ρ_a	Density of air corresponding to water temperature	g/cm^3	**0.0012** U.S. EPA OSW recommends this default value when site-specific information is not available, consistent with U.S. EPA (1994), both of which cite Weast (1979) as the source of this value. This value applies at standard conditions (298 K and 1 atm). There is no significant uncertainty associated with this variable.
ρ_w	Density of water corresponding to water temperature	g/cm^3	**1** U.S. EPA OSW recommends this default value, consistent with U.S. EPA (1994), both of which cite Weast (1979) as the source of this value. This value applies at standard conditions (298 K and 1 atm). There is no significant uncertainty associated with this variable.
k	von Karman's constant	unitless	**0.4** This value is a constant. U.S. EPA OSW recommends the use of this value, consistent with U.S. EPA (1994). The following uncertainty is associated with this variable: (1) The original source of this variable value is unknown. Therefore, any uncertainties associated with its use are also unknown.
λ_z	Dimensionless viscous sublayer thickness	unitless	**4** This value is site-specific. U.S. EPA OSW recommends the use of this default value when site-specific information is not available; consistent with U.S. EPA (1994).
μ_w	Viscosity of water corresponding to water temperature	g/cm-s	**0.0169** U.S. EPA OSW recommends this default value, consistent with U.S. EPA (1994), which both cite Weast (1979) as the source of this value. This value applies at standard conditions (298 K and 1 atm). There is no significant uncertainty associated with this variable.

TABLE B-2-14

LIQUID-PHASE TRANSFER COEFFICIENT (SURFACE WATER AND SEDIMENT EQUATIONS)

REFERENCES AND DISCUSSION

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units*. January.

This document is cited as one of the sources of the range of D_w values and assumed C_d, ρ_a, ρ_w, k, λ_z, and μ_w values of 0.0011, 1.2 x 10^{-3}, 1, 0.4, 4, and 1.69 x 10^{-2}, respectively. This document cites (1) Weast (1979) as its source of information regarding ρ_a, ρ_w, and μ_w; and (2) U.S. EPA (1993a) as its source of information regarding C_d, k, and d_z.

U.S. EPA. 1993a. *Addendum: Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. Working Group Recommendations. Office of Solid Waste and Office of Research and Development. Washington, D.C. September 24.

This document is cited by U.S. EPA (1994) and NC DEHNR (1997) as the source of the recommended drag coefficient (C_d) value of 0.0011 and the recommended von Karman's constant (k) value of 0.4. The original sources of variable values are not identified.

U.S. EPA. 1993b. *Addendum to Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. External Review Draft. Office of Solid Waste and Office of Research and Development. Washington, D.C. November 10.

This document recommends a value of 0.0011 for the drag coefficient (C_d) variable or a value of 0.4 for von Karman's constant (k). No sources are cited for these values.

U.S. EPA. 1994. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes*. *Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. Office of Emergency and Remedial Response. Office of Solid Waste. December 14.

This document is cited as one of the sources of the range of D_w values and assumed C_d, ρ_a, ρ_w, k, λ_z, and μ_w values of 0.0011, 1.2 x 10^{-3}, 1, 0.4, 4, and 1.69 x 10^{-2}, respectively. This document cites (1) Weast (1979) as its source of information regarding ρ_a, ρ_w, and μ_w; and (2) U.S. EPA (1993a) as its source of information regarding C_d, k, and d_z.

Weast, R. C. 1979. *CRC Handbook of Chemistry and Physics*. 60th ed. CRC Press, Inc. Cleveland, Ohio.

This document is cited as the source of ρ_a, ρ_w, and μ_w variables of 1.2 x10^{-3}, 1, and 1.69 x 10^{-2}, respectively.

TABLE B-2-15

GAS-PHASE TRANSFER COEFFICIENT
(SURFACE WATER AND SEDIMENT EQUATIONS)

Description

This equation calculates the rate of contaminant transfer from the gas phase for a flowing or quiescent system. Uncertainties associated with this equation include the following:

(1) Minimal or insignificant uncertainty is assumed to be associated with the variables D_a, μ_a, and ρ_a.
(2) No original sources were identified for equations used to derive recommended values or specific recommended values for variables C_d, k, and λ_z. Therefore, the degree and direction of any uncertainties associated with these variables are unknown.
(3) Uncertainties associated with the remaining variables are site-specific.

Equation

Flowing streams or rivers

$$K_G = 36{,}500 \ m/yr$$

Quiescent lakes or ponds

$$K_G = (C_d^{0.5} \cdot W) \cdot \left(\frac{k^{0.33}}{\lambda_z} \right) \cdot \left(\frac{\mu_a}{\rho_a \cdot D_a} \right)^{-0.67} \cdot 3.1536 \times 10^7$$

For mercury modeling:

The gas phase transfer coefficient is calculated for divalent mercury (Hg^{2+}) and methyl mercury (MHg) using their respective fate and transport parameters .

Variable	Description	Units	Value
K_G	Gas-phase transfer coefficient	m/yr	

TABLE B-2-15

GAS-PHASE TRANSFER COEFFICIENT
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
C_d	Drag coefficient	unitless	**0.0011** This variable is site-specific. U.S. EPA OSW recommends the use of this default value when site-specific information is not available, consistent with U.S. EPA (1993a; 1993b; 1994) and NC DEHNR (1997). The following uncertainty is associated with this variable: (1) The original source of this variable is unknown.
W	Average annual wind speed	m/s	**3.9** Consistent with U.S. EPA (1990), U.S. EPA OSW recommends a default value of 3.9 m/s. See Chapter 3 for guidance regarding the references and methods used to determine a site-specific value that isconsistent with air dispersion modeling. The following uncertainty is associated with this variable: To the extent that site-specific or local values for this variable are not available, default values may not accurately represent site-specific conditions. The uncertainty associated with the selection of a single value from within the range of windspeeds at a single location may be more significant than the uncertainty associated with choosing a single windspeed to represent all locations.
k	von Karman's constant	unitless	**0.4** This value is a constant. U.S. EPA OSW recommends the use of this value, consistent with U.S. EPA (1994). The following uncertainty is associated with this variable: (1) The original source of this variable is unknown.
λ_z	Dimensionless viscous sublayer thickness	unitless	**4** This value is site-specific. U.S. EPA OSW recommends the use of this default value when site-specific information is not available, consistent with U.S. EPA (1994). The following uncertainty is associated with this variable: (1) The original source of this variable is unknown.

TABLE B-2-15

GAS-PHASE TRANSFER COEFFICIENT
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
μ_a	Viscosity of air	g/cm-s	**1.81×10^{-4}** U.S. EPA OSW recommends the use of this value, based on Weast (1980). This is consistent with NC DEHNR (1997). This value applies at standard conditions (20 °C or 298 K and 1 atm, or 760 mm Hg). The following uncertainty is associated with this variable: (1) The viscosity of air may vary with temperature.
ρ_a	Density of air	g/cm^3	**0.0012** U.S. EPA OSW recommends the use of this value, based on Weast (1980); this is consistent with NC DEHNR (1997). This value applies at standard conditions (20 °C or 298 K and 1 atm, or 760 mm Hg). The following uncertainty is associated with this variable: (1) The density of air will vary with temperature.
D_a	Diffusivity of COPC in air	cm^2/s	**Varies (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC physical and chemical parameter tables in Appendix A-2. The following uncertainty is associated with this variable: (1) The recommended D_a values may not accurately represent the behavior of COPCs under water body-specific conditions. However, the degree of uncertainty is expected to be minimal.
3.1536×10^7	Units conversion factor	s/yr	

TABLE B-2-15

GAS-PHASE TRANSFER COEFFICIENT
(SURFACE WATER AND SEDIMENT EQUATIONS)

REFERENCES AND DISCUSSION

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units*. January.

This document is cited as one of the sources of the variables ρ_a, k, λ_z, and μ_a values of 1.2 x 10^{-3}, 0.4, 4, and 1.81 E-04, respectively. This document cites (1) Weast (1979) as its source of information for ρ_a and μ_a, and (2) U.S. EPA (1993a) as its source of information for k and λ_z.

U.S. EPA. 1993a. *Addendum: Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustion Emissions*. Working Group Recommendations. Office of Solid Waste, and Office of Research and Development. Washington, D.C. September 24.

This document is cited by U.S. EPA (1994) and NC DEHNR (1997) as the source of (1) the recommended drag coefficient (C_d) value of 0.0011, (2) the recommended von Karman's constant (k) value of 0.4, and (3) the recommended dimensionless viscous sublayer thickness (λ_z) value of 4. The original sources of these variable values are not identified.

U.S. EPA. 1993b. *Addendum to Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. External Review Draft. Office of Solid Waste, and Office of Research and Development. Washington, D.C. November 10.

This document recommends (1) a value of 0.0011 for the drag coefficient (C_d) variable, (2) a value of 0.4 for von Karman's constant (K), and (3) a value of 4 for the dimensionless viscous sublayer thickness (λ_z) variable. The original sources of the variable values are not identified.

U.S. EPA. 1994. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes*. *Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. Office of Emergency and Remedial Response. Office of Solid Waste. December 14.

This document is cited as one of the sources of the variables ρ_a, k, λ_z, and μ_a values of 1.2 x 10^{-3}, 0.4, 4, and 1.81 E-04, respectively. This document cites (1) Weast (1979) as its source of information for ρ_a and μ_a, and (2) U.S. EPA (1993a) as its source of information for k and λ_z.

Weast, R.C. 1979. *CRC Handbook of Chemistry and Physics.* 60th ed. CRC Pres, Inc. Cleveland, Ohio. This document is cited as the source of ρ_a, ρ_w, and μ_a variables of 1.2 x 10^{-3}, 1, and 1.69 x 10^{-2}, respectively.

TABLE B-2-16

BENTHIC BURIAL RATE CONSTANT
(SURFACE WATER AND SEDIMENT EQUATIONS)

Description

This equation calculates the constant for water column loss constant due to burial in benthic sediment.

Uncertainties associated with this equation include the following:

(1) All of the variables in Table B-2-16 are site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of K_b. The degree of uncertainty associated with each of these variables is as follows: (a) X_e—about one order of magnitude at the most, (b) BS, d_{bs}, Vf_x, TSS, and A_W—limited because of the narrow recommended ranges for these variables or because resources to estimate variable values are generally available, (c) A_L and SD—very site-specific, degree of uncertainty unknown.

Based on the possible ranges for the input variables to this equation, values of k_b can range over about one order of magnitude.

Equation

$$k_b = \left(\frac{X_e \cdot A_L \cdot SD \cdot 10^3 - Vf_x \cdot TSS}{A_W \cdot TSS} \right) \left(\frac{TSS \cdot 10^{-6}}{BS \cdot d_{bs}} \right)$$

Variable	Description	Units	Value
k_b	Benthic burial rate constant	yr^{-1}	
X_e	Unit soil loss	$kg/m^2\text{-}yr$	**Varies (calculated - Table B-2-7)** This variable is site-specific and is calculated by using the equation in Table B-2-7. The following uncertainty is associated with this variable: (1) All of the variables in the equation used to calculate unit soil loss, X_e, are site-specific. Use of default values rather than site-specific values, for any or all of the equation variables, will result in estimates of X_e that under- or overestimate the actual value. The degree or magnitude of any under- or overestimation is expected to be about one order of magnitude or less.

TABLE B-2-16

BENTHIC BURIAL RATE CONSTANT
(SURFACE WATER AND SEDIMENT EQUATIONS)

(Page 2 of 5)

Variable	Description	Units	Value
A_L	Total watershed area receiving deposition	m^2	**Varies (site-specific)** This variable is site-specific (see Chapter 4). Uncertainties associated with this variable are site-specific.
SD	Sediment delivery ratio	unitless	**Varies (calculated - Table B-2-8)** This variable is site-specific and is calculated by using the equation in Table B-2-8. Uncertainties associated with this variable include the following: (1) The default values for empirical intercept coefficient, *a*, recommended for use in the equation in Table B-2-8, are average values based on various studies of sediment yields from various watersheds. Therefore, these default values may not accurately represent site-specific watershed conditions. As a result, use of these default values may contribute to under- or overestimation of the benthic burial rate constant, k_b. (2) The default value for empirical slope coefficient, *b*, recommended for use in in the equation in Table B-2-8 is based on a review of sediment yields from various watersheds. This single default value may not accurately represent site-specific water shed conditions. As a result, use of this default value may contribute to under-or overestimation of k_b.
10^3	Units conversion factor	g/kg	
Vf_x	Average volumetric flow rate through water body	m^3/yr	**Varies (site-specific)** This variable is site-specific and should be an annual average value. The following uncertainty is associated with this variable: (1) Use of default average volumetric flow rate, Vf_x, values may not accurately represent site-specific water body conditions. Therefore, the use of such default values may contribute to the under- or overestimation of k_b. However, it is expected that the uncertainty associated with this variable will be limited, because resources such as maps, aerial photographs, and gauging station measurements—from which average volumetric flow rate through water body, Vf_x, can be estimated—are generally available.

TABLE B-2-16

BENTHIC BURIAL RATE CONSTANT
(SURFACE WATER AND SEDIMENT EQUATIONS)

(Page 3 of 5)

Variable	Description	Units	Value
TSS	Total suspended solids concentration	mg/L	**2 to 300** This variable is site-specific. U.S. EPA OSW recommends the use of site- and waterbody specific measured values, representative of long-term average annual values for the water body of concern (see Chapter 3). A value of 10 mg/L was cited by NC DEHNR (1997), U.S. EPA (1993a), and U.S. EPA (1993b) in the absense of site-specific measured data. The following uncertainty is associated with this variable: Limitation on measured data used for determining a water body specific total suspended solids (*TSS*) value may not accurately reflect site- and water body-specific conditions long term. Therefore, the *TSS* value may contribute to the under-or overestimation of f_{wc}.
A_W	Water body surface area	m^2 (average for the entire year)	**Varies (site-specific)** This variable is site-specific (see Chapter 4), and should be an average annual value. The units of this variable are presented as they are because the value selected is assumed to represent an average value for the entire year. Uncertainties associated with this variable are site-specific, and expected to be limited, because maps, aerial photographs ─and other resources from which water body surface area, A_W, can be measured─are readily available.
1×10^{-6}	Units conversion factor	kg/mg	
BS	Benthic solids concentration	g/cm^3 (equivalent to kg/L)	**1.0** This variable is site-specific. U.S. EPA OSW recommends a default value of 1.0, consistent with U.S. EPA (1993b), which states that this value should be reasonable for most applications. The recommended default value is also consistent with other U.S. EPA (1993a; 1993b; 1994) guidance. The following uncertainty is associated with this variable: (1) The recommended default benthic solids concentration, *BS*, value may not accurately represent site-specific water body conditions. Therefore, use of this default value may contribute to the under- or overestimation of k_b.

TABLE B-2-16

BENTHIC BURIAL RATE CONSTANT
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
d_{bs}	Depth of upper benthic sediment layer	m	**0.03** This variable is site-specific. U.S. EPA OSW recommends a default upper-benthic sediment depth of 0.03 meter, which is based on the center of this range cited by U.S. EPA (1993a; 1993b). This range is consistent with U.S. EPA (1994). The following uncertainty is associated with this variable: (1) The recommended default value for depth of upper benthic layer, d_{bs}, may not accurately represent site-specific water body conditions. Therefore, use of this default value may contribute to the under- or overestimation of k_b. However, the degree of uncertainty associated with this variable is expected to be limited because of the narrow recommended range.

TABLE B-2-16

BENTHIC BURIAL RATE CONSTANT
(SURFACE WATER AND SEDIMENT EQUATIONS)

REFERENCES AND DISCUSSION

NC DEHNR 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units.* January.

This document is cited as one of the sources of the range of all recommended specific *BS* and d_{bs} values, and the recommended *TSS* value. This document cites U.S. EPA (1993a) as its source.

U.S. EPA. 1993a. *Addendum: Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Working Group Recommendations. Office of Solid Waste, and Office of Research and Development. Washington, D.C. September 24.

This document is cited by U.S. EPA (1994) and NC DEHNR (1997) as the source of (1) the *TSS* value, (2) the range and recommended *BS* value, and (3) the range and recommended depth of upper benthic layer (d_{bs}) value.

U.S. EPA 1993b. *Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. External Review Draft. Office of Research and Development. Washington, D.C. November.

This document states that the upper benthic sediment depth, d_{bs}, representing the portion of the bed in equilibrium with the water column, cannot be precisely specified. However, the document states that values from 0.01 to 0.05 meter would be appropriate. This document also recommends a *TSS* value of 10 mg/L and a specific benthic solids concentration (*BS*) value.

U.S. EPA 1994. *Draft Guidance for Performing Screening Level Risk Analyses at Combustor Facilities Burning Hazardous Waste*. *Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. April 15.

This document is cited as one of the reference sources for the d_{bs} value. The recommended value is the midpoint of an acceptable range. This document is also cited as one of the reference source documents for the default *BS* value. This document cites U.S. EPA (1993a) as its source.

TABLE B-2-17

TOTAL WATER COLUMN CONCENTRATION
(SURFACE WATER AND SEDIMENT EQUATIONS)

Description

This equation calculates the total water column concentration of COPCs; this includes both dissolved COPCS and COPCs sorbed to suspended solids.

Uncertainties associated with this equation include the following:

(1) All of the variables in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}.

The degree of uncertainty associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wtot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, the uncertainty associated with using default *OC* values may be significant in specific cases.

Equation

$$C_{wctot} = f_{wc} \cdot C_{wtot} \cdot \frac{d_{wc} + d_{bs}}{d_{wc}}$$

For mercury modeling:

Total water column concentration is calculated for divalent mercury (Hg^{2+}) and methyl mercury (MHg) using their respective C_{wtot} values and f_{wc} values.

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg/L	

TABLE B-2-17

TOTAL WATER COLUMN CONCENTRATION
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
f_{wc}	Fraction of total water body COPC concentration in the water column	unitless	**0 to 1 (calculated - Table B-2-10)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-10. The following uncertainty is associated with this variable: (1) The default variable values recommended for use in Table B-2-10 may not accurately represent site-specific water body conditions. However, the ranges of several variables—including d_{bs}, and θ_{bs} - is relatively narrow; therefore, the uncertainty is expected to be relatively small. Other variables, such as d_{wc} and d_z, can be reasonably estimated on the basis of generally available information. The largest degree of uncertainty may be introduced by the default medium specific *OC* content values. *OC* content values are often not readily available and can vary widely for different locations in the same medium. Therefore, default values may not adequately represent site-specific conditions.
C_{wtot}	Total water body COPC concentration, including water column and bed sediment	mg/L	**Varies (calculated - Table B-2-9)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-9. The following uncertainty is associated with this variable: (1) The default variable values recommended for use in the equation in Table B-2-9 may not accurately represent site--specific water body conditions. The degree of uncertainty associated with variables Vf_x, A_w, d_{wc}, and d_{bs} is expected to be limited either because the probable ranges for variables are narrow or information allowing accurate estimates is generally available. Uncertainty associated with f_{wc} is largely the result of water body associated with default *OC* content values, and may be significant in specific instances. Uncertainties associated with the total COPC load into water body (L_T) and overall total water body COPC dissipation rate constant (k_{wt}) may also be significant in some instances because of the summation of many variable-specific uncertainties.

TABLE B-2-17

TOTAL WATER COLUMN CONCENTRATION
(SURFACE WATER AND SEDIMENT EQUATIONS)

(Page 3 of 4)

Variable	Description	Units	Value
d_{wc}	Depth of water column	m	**Varies (site-specific)** This variable is site-specific, and should be an average annual value. The following uncertainty is associated with this variable: (1) Use of default values for depth of water column, d_{wc}, may not accurately reflect site-specific water body conditions. Therefore, use of default values may contribute to the under- or overestimation of C_{wctot}. However, the degree of uncertainty associated with this variable is expected to be limited, because information regarding this variable is generally available.
d_{bs}	Depth of upper benthic sediment layer	m	**0.03** This variable is site-specific. U.S. EPA OSW recommends a default upper-benthic sediment depth of 0.03 meter, which is based on the center of this range cited by U.S. EPA (1993a; 1993b) This range is consistent with U.S. EPA (1994). The following uncertainty is associated with this variable: (1) The recommended default value for depth of upper benthic layer, d_{bs}, may not accurately represent site-specific water body conditions. Therefore, use of this default value may contribute to the under- or overestimation of C_{wctot}. However, the degree of uncertainty associated with this variable is expected to be limited because of the narrow recommended range.

TABLE B-2-17

TOTAL WATER COLUMN CONCENTRATION
(SURFACE WATER AND SEDIMENT EQUATIONS)

REFERENCES AND DISCUSSION

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units.* January.

This document is cited as one of the sources of the range of d_{bs} values. This document cites U.S. EPA (1993a) as its source.

U.S. EPA. 1993a. *Addendum: Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Working Group Recommendations. Office of Solid Waste and Office of Research and Development. Washington, D.C. September 24.

This document is cited by U.S. EPA (1994) and NC DEHNR (1997) as one of the sources of the ranges of d_{bs} values. No original source of this range was identified.

U.S. EPA. 1993b. *Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* External Review Draft. Office of Research and Development. Washington, D.C. November.

This document states that the upper benthic sediment depth, d_{bs}, representing the portion of the bed in equilibrium with the water column, cannot be precisely specified. However, the document states that values from 0.01 to 0.05 meter would be appropriate.

U.S. EPA. 1994. *Draft Guidance for Performing Screening Level Risk Analyses at Combustor Facilities Burning Hazardous Waste. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facility*. April 15.

This document is cited as one of the reference sources for the default value for depth of upper benthic layer (d_{bs}). The recommended value is the midpoint of an acceptable range. This document cites U.S. EPA (1993a) as the source of its information. The degree of uncertainty associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating these variables is generally available (d_{wc}) or the probable range for a variable (d_{bs}) is narrow. Uncertainty associated with the variables f_{wc} and C_{wtot} is largely associated with the use of default *OC* content values. Because *OC* content is known to vary widely in different locations in the same medium, use of default medium-specific values can result in significant uncertainty in some instances.

TABLE B-2-18

DISSOLVED PHASE WATER CONCENTRATION (SURFACE WATER AND SEDIMENT EQUATIONS)

Description

This equation calculates the concentration of contaminant dissolved in the water column.

Uncertainties associated with this equation include the following:

(1) The variables in Table B-2-18 are site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{dw}. The uncertainty associated with the variables C_{wCTOT} and Kd_{sw} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, using default *OC* values may result in significant uncertainty in specific cases.

Equation

$$C_{dw} = \frac{C_{wctot}}{1 + Kd_{sw} \cdot TSS \cdot 10^{-6}}$$

For mercury modeling:

Dissolved phase water concentration is calculated for divalent mercury (Hg^{2+}) and methyl mercury (MHg) using their respective C_{wctot} values and Kd_{sw} values.

Variable	Description	Units	Value
C_{dw}	Dissolved phase water concentration	mg/L	
10^{-6}	Units conversion factor	kg/mg	

TABLE B-2-18

DISSOLVED PHASE WATER CONCENTRATION
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg/L	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-17. The following uncertainty is associated with this variable: (1) All of the variables in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. The degree of uncertainty associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wtot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, using default *OC* values may result in significant uncertainty in specific cases.
Kd_{sw}	Suspended sediments/surface water partition coefficient	L/kg	**Varies (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-2. The following uncertainty is associated with this variable: (1) Values contained in Appendix A-2 for Kd_{sw} are based on default *OC* content values for surface water and soil. Because OC content can vary widely for different locations in the same medium, the uncertainty associated with estimated Kd_{sw} values based on default *OC* content values may be significant in specific cases.
TSS	Total suspended solids concentration	mg/L	**2 to 300** This variable is site-specific. U.S. EPA OSW recommends the use of site- and waterbody specific measured values, representative of long-term average annual values for the water body of concern (see Chapter 5). A value of 10 mg/L was cited by NC DEHNR (1997), U.S. EPA (1993a), and U.S. EPA (1993b) in the absense of site-specific measured data. The following uncertainty is associated with this variable: Limitation on measured data used for determining a water body specific total suspended solids (*TSS*) value may not accurately reflect site- and water body-specific conditions long term. Therefore, the *TSS* value may contribute to the under-or overestimation of f_{wc}.

TABLE B-2-18

DISSOLVED PHASE WATER CONCENTRATION
(SURFACE WATER AND SEDIMENT EQUATIONS)

(Page 3 of 3)

REFERENCES AND DISCUSSION

NC DEHNR 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units.* January.

This document is cited as one of the sources for Kd_s values and a default *TSS* value of 10. This document cites (1) U.S. EPA (1993a; 1993b) as its sources of information regarding *TSS*, and (2) RTI (1992) as its source regarding Kd_s.

U.S. EPA. 1993a. *Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Working Group Recommendations. Office of Solid Waste and Office of Research and Development. Washington, D.C. September 24.

This document is cited by U.S. EPA (1994) and NC DEHNR (1997) as one of the sources of the range of Kd_s value and the assumed *OC* value of 0.075 for surface water. The generic equation for calculating partition coefficients (soil, surface water, and bed sediments) is as follows: $Kd_{ij} = K_{ocj} * OC_i$. K_{oc} is a chemical-specific value; however, *OC* is medium-specific. The range of Kd_s values was based on an assumed *OC* value of 0.01 for soil. Therefore, the Kd_{sw} values were estimated by multiplying the Kd_s values by 7.5, because the *OC* value for surface water is 7.5 times greater than the *OC* value for soil. This document is also cited by U.S. EPA (1994) and NC DEHNR (1997) as the source of the recommended *TSS* value.

U.S. EPA. 1993b. *Addendum: Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* External Review Draft. Office of Research and Development. November.

This document is cited by U.S. EPA (1994) and NC DEHNR (1997) as one of the sources of the range of Kd_s value and the assumed *OC* value of 0.075 for surface water. The generic equation for calculating partition coefficients is as follows: $Kd_{ij} = K_{ocj} * OC_i$. K_{oc} is a chemical-specific value; however, *OC* is medium-specific. The range of Kd_s values was based on an assumed *OC* value of 0.01 for soil. Therefore, the Kd_{sw} values were estimated by multiplying the Kd_s values by 7.5, because the *OC* value for surface water is 7.5 times greater than the *OC* value for soil. This document is also cited by U.S. EPA (1994) and NC DEHNR (1997) as the source of the recommended *TSS* value.

U.S. EPA. 1994. *Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Waste*. *Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. April 15.

This document is cited as one of the sources of the range of Kd_s values, citing RTI (1992) as its source of information.

TABLE B-2-19

COPC CONCENTRATION IN BED SEDIMENT (SURFACE WATER AND SEDIMENT EQUATIONS)

(Page 1 of 4)

Description

This equation calculates the COPC concentration in bed sediments.

Uncertainties associated with this equation include the following:

(1) The default variable values recommended for use in the equation in Table B-2-19 may not accurately represent site-specific water body conditions. The degree of uncertainty associated with variables θ_{bs}, BS, d_{wc}, and d_{bs} is expected to be limited either because the probable ranges for these variables are narrow or because information allowing reasonable estimates is generally available.

(2) Uncertainties associated with variables f_{bs}, C_{wtot} and Kd_{bs} are largely associated with the use of default OC content values in their calculation. The uncertainty may be significant in specific instances, because OC content is known to vary widely in different locations in the same medium.

Equation

$$C_{sed} = f_{bs} \cdot C_{wtot} \cdot \frac{Kd_{bs}}{\theta_{bs} + Kd_{bs} \cdot BS} \cdot \frac{d_{wc} + d_{bs}}{d_{bs}}$$

For mercury modeling':

COPC concentration in bed sediment is calculated for divalent mercury (Hg^{2+}) and methyl mercury (MHg) using their respective C_{wtot} values; f_{bs} values; and Kd_{bs} values.

Variable	Description	Units	Value
C_{sed}	COPC concentration in bed sediment	mg/kg	
f_{bs}	Fraction of total water body COPC concentration in benthic sediment	unitless	**Varies (calculated - Table B-2-10)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-10. The following uncertainty is associated with this variable: (1) The default values for the variables in Table B-2-10 may not accurately represent site- and water body-specific conditions. However, the range of several variables—including d_{bs}, BS, and θ_{bs}—is relatively narrow. Other variables, such as d_{wc} and d_z, can be reasonably estimated on the basis of generally available information. The largest degree of uncertainty may be introduced by the default medium-specific OC content values. Because OC content values may vary widely in different locations in the same medium, by using default values may result in significant uncertainty in specific cases.

TABLE B-2-19

COPC CONCENTRATION IN BED SEDIMENT
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
C_{wtot}	Total water body COPC concentration, including water column and bed sediment	mg/L	**Varies (calculated - Table B-2-9)** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-9. The following uncertainty is associated with this variable: (1) The default variable values recommended for use in the equation in Table B-2-9 may not accurately represent site--specific water body conditions. The degree of uncertainty associated with variables Vf_x, A_W, d_{wc}, and d_{bs} is expected to be limited either because the probable ranges for these variables are narrow or information allowing reasonable estimates is generally available. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values and may be significant in specific instances. Uncertainties associated with the variable L_T and k_{wt} may also be significant because of the summation of many variable-specific uncertainties.
Kd_{bs}	Bed sediment/sediment pore water partition coefficient	L/kg	**Varies (see Appendix A-2)** This variable is COPC-specific, and should be determined from the COPC tables in Appendix A-2. The following uncertainty is associated with this variable: (1) The default range (8 to 2,100,000 L/kg) of Kd_{bs} values are based on default OC content values for sediment and soil. Because medium-specific OC content may vary widely at different locations in the same medium, the uncertainty associated with Kd_{bs} values calculated by using default OC content values may be significant in specific instances.
θ_{bs}	Bed sediment porosity	$L_{water}/L_{sediment}$	**0.4 to 0.8** **Default: 0.6** This variable is site-specific. U.S. EPAOSW recommends a default bed sediment porosity of 0.6 (by using a BS value of 1 g/cm^3 and a solids density [ρ_s] value of 2.65 kg/L), calculated by using the following equation (U.S. EPA 1993a): $\theta_{bs} = 1 - BS / \rho_s$ This is consistent with other U.S. EPA (1993b and 1994) guidance. The following uncertainty is associated with this variable: (1) To the extent that the recommended default values of BS and ρ_s do not accurately represent site- and water body-specific conditions, θ_{bs} will be under- or overestimated to some degree. However, the degree of uncertainty is expected to be minimal, based on the narrow range of recommended values.

TABLE B-2-19

COPC CONCENTRATION IN BED SEDIMENT
(SURFACE WATER AND SEDIMENT EQUATIONS)

Variable	Description	Units	Value
BS	Benthic solids concentration	g/cm^3	**0.5 to 1.5** **Default: 1.0** This variable is site-specific. U.S. EPA OSW recommends a default value of 1.0, consistent with U.S. EPA (1993a), which states that this value should be reasonable for most applications. No reference is cited for this recommendation. This is also consistent with other U.S. EPA (1993b and 1994) guidance. The following uncertainty is associated with this variable: (1) The recommended default value for *BS* may not accurately represent site- and water body-specific conditions. Therefore, the variable *Csed* may be under- or overestimated to a limited degree, as indicated by the narrow range of recommended values.
d_{wc}	Depth of water column	m	**Varies (site-specific)** This variable is site-specific. The following uncertainty is associated with this variable: (1) Use of default d_{wc} values may not accurately reflect site-specific conditions. Therefore, use of these default values may contribute to the under- or overestimation of the variable C_{sed}. However, the degree of uncertainty is expected to be minimal, because resources allowing reasonable water body-specific estimates of d_{wc} are generally available.
d_{bs}	Depth of upper benthic sediment layer	m	**0.03** This variable is site-specific. U.S. EPA recommends a default upper-benthic sediment depth of 0.03 meter, which is based on the center of this range cited by U.S. EPA (1993b). This is consistent with U.S. EPA (1994) and NC DEHNR (1997). The following uncertainty is associated with this variable: (1) Use of default d_{bs} values may not accurately reflect site-specific conditions. Therefore, use of these values may contribute to the under- or overestimation of the variable C_{sed}. However, the degree of uncertainty is expected to be small, based on the narrow recommended range of default values.

TABLE B-2-19

COPC CONCENTRATION IN BED SEDIMENT
(SURFACE WATER AND SEDIMENT EQUATIONS)

REFERENCES AND DISCUSSION

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units.* January.

This document is cited as one of the reference source documents for the default value for bed sediment porosity (θ_{bs}). This document cites U.S. EPA (1993a; 1993b) as its source of information. This document is also cited as one of the reference source documents for the default value for depth of the upper benthic layer. The default value is the midpoint of an acceptable range. This document cites U.S. EPA (1993a; 1993b) as its source of information for the range of values for the depth of the upper benthic layer. This document is also cited as one of the reference source documents for the default benthic solids concentration (*BS*).

U.S. EPA. 1993a. *Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* External Review Draft. Office of Research and Development. Washington, D.C. November 1993.

This document is cited by U.S. EPA (1994) and NC DEHNR (1997) as one of the sources of the range of Kd_s values and an assumed *OC* value of 0.04 for sediment. The generic equation for calculating partition coefficients (soil, surface water, and bed sediments) is as follows: $Kd_{ij} = K_{oc} * OC_i$. K_{oc} is a chemical-specific value; however, *OC* is medium-specific. The range of Kd_s values was based on an assumed *OC* value of 0.01 for soil. Therefore, the Kd_{bs} value was estimated by multiplying the Kd_s values by 4, because the *OC* value for sediment is four times greater than the *OC* value for soil. This document is also cited as the source of the equation for calculating bed sediment porosity (θ_{bs}). No source of this equation was identified. This document was also cited as the source for the range of the benthic solids concentration (*BS*). No source of this range was identified.

U.S. EPA. 1993b. *Addendum: Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Working Group Recommendations. Office of Solid Waste and Office of Research and Development. Washington, D.C. September 24.

This document is cited by NC DEHNR (1997) and U.S. EPA (1994) as the source of the default bed sediment porosity value (θ_{bs}), the default benthic solids concentration value (*BS*), and the range for depth of upper benthic layer (d_{bs}) values.

U.S. EPA. 1994. *Draft Guidance for Performing Screening Level Risk Analyses at Combustor Facilities Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. April 15.

This document is cited as one of the sources of the range of Kd_s values and an assumed *OC* value of 0.04 for sediment. This document cites RTI (1992) as its source of information regarding Kd_s values. This document is cited as one of the reference source documents for the default value for bed sediment porosity (θ_{bs}). This document cites U.S. EPA (1993a; 1993b) as its source. This document is also cited as one of the reference source documents for the default value for depth of upper benthic layer (d_{bs}). The default value is the midpoint of an acceptable range. This document cites U.S. EPA (1993a; 1993b) as its source of information for the range of values for the depth of the upper benthic layer. This document is also cited as one of the reference source documents for the default benthic solids concentration (*BS*).

TABLE B-3-1

PLANT CONCENTRATION DUE TO DIRECT DEPOSITION
(TERRESTRIAL PLANT EQUATIONS)

Description

This equation calculates the COPC concentration in plants, resulting from wet and dry deposition of particle phase COPCs onto the exposed plant surface.

The limitations and uncertainty associated with calculating this value include the following:

(1) Uncertainties associated with the variables *Q*, *Dydp*, and *Dywp* are site-specific.
(2) The calculation of *kp* values does not consider chemical degradation processes. Inclusion of chemical degradation process would decrease the amount of time that a compound remains on plant surfaces (half-time) and thereby increase *kp* values. *Pd* decreases with increased *kp* values. Reduction of half-time from the assumed 14 days to 2.8 days, for example, would decrease *Pd* about 5-fold.
(3) The calculation of other parameter values (for example, *Fw* and *Rp*) is based directly or indirectly on studies of specific types of vegetation (primarily grasses and forbes). To the extent that the calculated parameter values do not accurately represent all site-specific forage species, uncertainty is introduced.
(4) The uncertainties associated with the variables F_v, *Tp*, and *Yp* are not expected to be significant.

Equation

$$Pd = \frac{1000 \cdot Q \cdot (1 - F_v) \cdot [Dydp + (Fw \cdot Dywp)] \cdot Rp \cdot [1.0 - \exp(-kp \cdot Tp)] \cdot 0.12}{Yp \cdot kp}$$

For mercury modeling:

$$Pd_{Mercury} = \frac{1000 \cdot (0.48 Q_{TotalMercury}) \cdot (1 - F_{v_{Hg^{2+}}}) \cdot [Dydp + (Fw \cdot Dywp)] \cdot Rp \cdot [1.0 - \exp(-kp \cdot Tp)] \cdot 0.12}{Yp \cdot kp}$$

In calculating *Pd* for mercury comounds, *Pd(Mercury)* is calculated as shown above using the total mercury emission rate (*Q*) measured at the stack and F_v for mercuric chloride (F_v = 0.85). As presented below, the calculated *Pd(Mercury)* value is apportioned into the divalent mercury (Hg^{2+}) and methyl mercury (MHg) forms based on a 78% Hg^{2+} and 22% MHg speciation split in plants (see Chapter 2).

Pd (Hg^{2+}) = 0.78 *Pd(Mercury)*
Pd (MHg) = 0.22 *Pd(Mercury)*

After calculating species specific *Pd* values, divalent and methyl mercury should continue to be modeled throughout Appendix B equations as individual COPCs.

TABLE B-3-1

PLANT CONCENTRATION DUE TO DIRECT DEPOSITION (TERRESTRIAL PLANT EQUATIONS)

Variable	Description	Units	Value
Pd	Plant concentration due to direct deposition	mg/kg WW	
1000	Units conversion factor	mg/g	
Q	COPC-specific emission rate	g/s	**Varies (site-specific)** This value is COPC- and site-specific (see Chapters 2 and 3). Uncertainties associated with this variable are also COPC- and site-specific.
F_v	Fraction of COPC air concentration in vapor phase	unitless	**0 to 1 (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-2. Uncertainties associated with this variable include the following: (1) Calculation is based on an assumption of a default S_T value for background plus local sources, rather than an S_T value for urban sources. If a specific site is located in an urban area, the use of the latter S_T value may be more appropriate. Specifically, the S_T value for urban sources is about one order of magnitude greater than that for background plus local sources and would result in a lower calculated F_v value; however, the F_v value is likely to be only a few percent lower. (2) According to Bidleman (1988), the equation used to calculate F_v assumes that the variable *c* is constant for all chemicals; however, the value of *c* depends on the chemical (sorbate) molecular weight, the surface concentration for monolayer coverage, and the difference between the heat of desorption from the particle surface and the heat of vaporization of the liquid-phase sorbate. To the extent that site- or COPC-specific conditions may cause the value of *c* to vary, uncertainty is introduced if a constant value of *c* is used to calculate F_v.
Dydp	Unitized yearly average dry deposition from particle phase	s/m^2-yr	**Varies (modeled)** This variable is COPC- and site-specific, and is determined by air dispersion modeling (see Chapter 3). Uncertainties associated with this variable are site-specific.

TABLE B-3-1

PLANT CONCENTRATION DUE TO DIRECT DEPOSITION
(TERRESTRIAL PLANT EQUATIONS)

Variable	Description	Units	Value
Rp	Interception fraction of the edible portion of plant	unitless	**0.5** U.S. EPA OSW recommends the use of the *Rp* value of 0.5 , which is consistent with the value used by U.S. EPA (1994b; 1995) in development of values for the fraction of deposition that adheres to plant surfaces, *Fw*, for forage. As summarized in Baes, Sharp, Sjoreen, and Shor (1984), experimental studies of pasture grasses identified a correlation between initial *Rp* values and productivity (standing crop biomass [*Yp*]) (Chamberlain 1970): $$Rp = 1 - e^{-\gamma \cdot Yp}$$ where: *Rp* = Interception fraction of edible portion of plant (unitless) γ = Empirical constant; Chamberlain (1970) presents a range of 2.3 to 3.3; Baes, Sharp, Sjoreen, and Shor (1984) uses the midpoint, 2.88, for pasture grasses. *Yp* = Yield or standing crop biomass (productivity) (kg DW/m^2) Baes, Sharp, Sjoreen, and Shor (1984) proposed using the same empirical relationship developed by Chamberlain (1970) for other vegetation classes. Class-specific estimates of the empirical constant, γ, were developed by forcing an exponential regression equation through several points, including average and theoretical maximum estimates of *Rp* and *Yp* (Baes, Sharp, Sjoreen, and Shor 1984). Uncertainties associated with this variable include the following: (1) The empirical relationship developed by Chamberlain (1970) on the basis of a study of pasture grass may not accurately represent all forage varieties of plants. (2) The empirical constants developed by Baes, Sharp, Sjoreen, and Shor (1984) for use in the empirical relationship developed by Chamberlain (1970) may not accurately represent site-specific mixes of plants.

TABLE B-3-1

PLANT CONCENTRATION DUE TO DIRECT DEPOSITION
(TERRESTRIAL PLANT EQUATIONS)

Variable	Description	Units	Value
Fw	Fraction of COPC wet deposition that adheres to plant surfaces	unitless	**Anions: 0.20** **Cations and most Organics: 0.6** Consistent with U.S. EPA (194b; 1995) in evaluating aboveground forage, U.S. EPA OSW recommends using the value of 0.2 for anions and 0.6 for cations and most organics. These values are the best available information, based on a review of the current scientific literature, with the following exception: U.S. EPA OSW recommends using an *Fw* value of 0.2 for the three organic COPC that ionize to anionic forms. These include (1) 4-chloroaniline, (2) n-nitrosodiphenylamine, and (3) n-nitrosodi-n-proplyamine (see Appendix A-2). The values estimated by U.S. EPA (1994b; 1995) are based on information presented in Hoffman, Thiessen, Frank, and Blaylock (1992), which presented values for a parameter (*r*) termed the "interception fraction." These values were based on a study in which soluble radionuclides and insoluble particles labeled with radionuclides were deposited onto pasture grass (specifically a combination of fescues, clover, and old field vegitation) via simulated rain. The parameter (*r*) is defined as "the fraction of material in rain intercepted by vegetation and initially retained" or, essentially, the product of *Rp* and *Fw*, as defined for use in this guidance: $r = Rp \cdot Fw$ The *r* values developed by Hoffman, Thiessen, Frank, and Blaylock (1992) were divided by an *Rp* value of 0.5 for forage (U.S. EPA 1994b). The *Fw* values developed by U.S. EPA (1994b) are 0.2 for anions and 0.6 for cations and insoluble particles. U.S. EPA (1994b; 1995) recommended using the *Fw* value calculated by using the *r* value for insoluble particles to represent organic compounds; however, no rationale for this recommendation is provided. Uncertainties associated with this variable include the following: (1) Values of *r* developed experimentally for pasture grass (specifically a combination of fescues, clover, and old field vegitation) may not accurately represent all forage varieties specificto a site. (2) Values of *r* assumed for most organic compounds, based on the behavior of insoluble polystryene microspheres tagged with radionuclides, may not accurately represent the behavior of organic compounds under site-specific conditions.
Dywp	Unitized yearly average wet deposition from particle phase	s/m^2-yr	**Varies (modeled)** This variable is COPC- and site-specific, and is determined by air dispersion modeling (see Chapter 3). Uncertainties associated with this variable are site-specific.

TABLE B-3-1

PLANT CONCENTRATION DUE TO DIRECT DEPOSITION
(TERRESTRIAL PLANT EQUATIONS)

Variable	Description	Units	Value
kp	Plant surface loss coefficient	yr^{-1}	**18** U.S. EPA OSW recommends the *kp* value of 18 recommended by U.S. EPA (1993; 1994b). The *kp* value selected is the midpoint of a possible range of values. U.S. EPA (1990) identified several processes—including wind removal, water removal, and growth dilution—that reduce the amount of contaminant that has been deposited on a plant surface. The term *kp* is a measure of the amount of contaminant lost to these physical processes over time. U.S. EPA (1990) cited Miller and Hoffman (1983) for the following equation used to estimate *kp*: $kp = (\ln 2 / t_{1/2}) \cdot 365 \text{ days/yr}$ where: $t_{1/2}$ = half-time (days) Miller and Hoffman (1983) report half-time values ranging from 2.8 to 34 days for a variety of contaminants on herbaceous vegetation. These half-time values result in *kp* values of 7.44 to 90.36 yr^{-1}. U.S. EPA (1993; 1994b) recommend a *kp* value of 18, based on a generic 14-day half-time, corresponding to physical processes only. The 14-day half-time is approximately the midpoint of the range (2.8 to 34 days) estimated by Miller and Hoffman (1983). Uncertainties associated with this variable include the following: (1) Calculation of *kp* does not consider chemical degradation processes. The addition of chemical degradation processes would decrease half-times and thereby increase *kp* values; plant concentration decreases as *kp* increases. Therefore, use of a *kp* value that does not consider chemical degradation processes is conservative. (2) The half-time values reported by Miller and Hoffman (1983) may not accurately represent the behavior of all COPCs on plants. (3) Based on this range (7.44 to 90.36), plant concentrations could range from about 1.8 times higher to about 5 times lower than the plant concentrations, based on a *kp* value of 18.

TABLE B-3-1

PLANT CONCENTRATION DUE TO DIRECT DEPOSITION
(TERRESTRIAL PLANT EQUATIONS)

(Page 6 of 10)

Variable	Description	Units	Value
Tp	Length of plant exposure to deposition per harvest of edible portion of plant	yr	**0.12** This variable is site-specific. U.S. EPA OSW recommends the use of these default values in the absence of site-specific information. U.S. EPA (1990), U.S. EPA (1994b), and NC DEHNR (1997) recommended treating *Tp* as a constant, based on the average periods between successive hay harvests and successive grazing. For forage, the average of the average period between successive hay harvests (60 days) and the average period between successive grazing (30 days) is used (that is, 45 days). *Tp* is calculated as follows: Tp = (60 days + 30 days)/ 2 ÷ 365 days/yr = 0.12 yr These average periods are from Belcher and Travis (1989), and are used when calculating the COPC concentration in cattle forage. The following uncertainty is associated with this variable: (1) Beyond the time frame of about 3 months for harvest cycles, if the *kp* value remains unchanged at 18, higher *Tp* values will have little effect on predicted COPC concentrations in plants.
0.12	Dry weight to wet weight conversion factor	unitless	**0.12** U.S. EPA OSW recommends using the value of 0.12. This default value is based on the average rounded value from the range of 80 to 95 percent water content in herbaceous plants and nonwoody plant parts (Taiz at al. 1991). The following uncertainty is associated with this variable: (1) The plant species considered in determining the default value may be different from plant varieties actually present at a site.

TABLE B-3-1

PLANT CONCENTRATION DUE TO DIRECT DEPOSITION (TERRESTRIAL PLANT EQUATIONS)

(Page 7 of 10)

Variable	Description	Units	Value
Yp	Yield or standing crop biomass of the edible portion of the plant (productivity)	kg DW/m^2	**0.24** U.S. EPA OSW recommends using the *Yp* value of 0.24. This default value is consistent with values presented in U.S. EPA (1994b) for forage (weighted average of pasture grass and hay *Yp* values determined in considering ingestion by an herbivorous mammal [cattle]), and with the resulting Rp value (see Table B-3-1) as determined by correlation with productivity (standing crop biomass [*Yp*]) (Chamberlain 1970). Based on a review of the currently available literature, this value appears to be based on the most complete and thorough information. The following uncertainty is associated with this variable: (1) The plant species considered in determining the default value for forage may be different from plant varieties actually present at a site. This may under- or overestimate *Yp*.

REFERENCES AND DISCUSSION

Baes, C.F., R.D. Sharp, A.L. Sjoreen, and R.W. Shor. 1984. *Review and Analysis of Parameters and Assessing Transport of Environmentally Released Radionuclides through Agriculture*. ORNL-5786. Oak Ridge National Laboratory. Oak Ridge, Tennessee. September.

This document proposed using the same empirical relationship developed by Chamberlain (1970) for other vegetation classes. Class-specific estimates of the empirical constant, γ, were developed by forcing an exponential regression equation through several points, including average and theoretical maximum estimates of *Rp* and *Yp*.

Belcher, G.D., and C.C. Travis. 1989. "Modeling Support for the RURA and Municipal Waste Combustion Projects: Final Report on Sensitivity and Uncertainty Analysis for the Terrestrial Food Chain Model." Interagency Agreement No. 1824-A020-A1, Office of Risk Analysis, Health and Safety Research Division, Oak Ridge National Laboratory. Oak Ridge, Tennessee. October.

This document recommends *Tp* values based on the average period between successive hay harvests and successive grazing.

Bidleman, T.F. 1988. "Atmospheric Processes." *Environmental Science and Technology*. Volume 22. Pages 361-367. November 4.

This document is cited by U.S. EPA (1994a) and NC DEHNR (1997) as the source of the equations for calculating F_v.

Chamberlain, A.C. 1970. "Interception and Retention of Radioactive Aerosols by Vegetation." *Atmospheric Environment*. 4:57 to 78.

Experimental studies of pasture grasses identified a correlation between initial *Rp* values and productivity (standing crop biomass [*Yp*]):

Rp	=	$1-e^{-\gamma \times Yp}$
γ	=	Empirical constant; range provided as 2.3 to 3.3
Yp	=	Standing crop biomass (productivity) (kg DW/m^2)

Hoffman, F.O., K.M. Thiessen, M.L. Frank, and B.G. Blaylock. 1992. "Quantification of the Interception and Initial Retention of Radioactive Contaminants Deposited on Pasture Grass by Simulated Rain." *Atmospheric Environment*. Vol. 26A. 18:3313 to 3321.

This document developed values for a parameter (*r*) that it termed "interception fraction," based on a study in which soluble gamma-emitting radionuclides and insoluble particles tagged with gamma-emitting radionuclides were deposited onto pasture grass (specifically, a combination of fescues, clover, and old field vegetation, including fescue) via simulated rain. The parameter, *r*, is defined as "the fraction of material in rain intercepted by vegetation and initially retained" or, essentially, the product of *Rp* and *Fw*, as defined by this guidance:

$$r = Rp \cdot Fw$$

Experimental *r* values obtained include the following:

- A range of 0.006 to 0.3 for anions (based on the soluble radionuclide iodide-131 [^{131}I]); when calculating *Rp* values for anions, U.S. EPA (1994a) used the highest geometric mean *r* value (0.08) observed in the study.

- A range of 0.1 to 0.6 for cations (based on the soluble radionuclide beryllium-7 [7Be]; when calculating *Rp* values for cations, U.S. EPA (1994a) used the highest geometric mean *r* value (0.28) observed in the study.

- A geometric range of values from 0.30 to 0.37 for insoluble polystyrene microspheres (IPM) ranging in diameter from 3 to 25 micrometers, labeled with cerium-141 [^{141}Ce], [^{95}N]b, and strontium-85 ^{85}Sr; when calculating *Rp* values for organics (other than three organics that ionize to anionic forms: 4-chloroaniline; n-nitrosodiphenylamine; and n-nitrosodi-n-propylamine, ─see Appendix A-2), U.S. EPA (1994a) used the geometric mean *r* value for IPM with a diameter of 3 micrometers. However, no rationale for this selection was provided.

The authors concluded that, for the soluble ^{131}I anion, interception fraction *r* is an inverse function of rain amount, whereas for the soluble cation ^{7}Be and the IPMs, *r* depends more on biomass than on amount of rainfall. The authors also concluded that (1) the anionic ^{131}I is essentially removed with the water after the vegetation surface has become saturated, and (2) the cationic ^{7}Be and the IPMs are adsorbed to, or settle out on, the plant surface. This discrepancy between the behavior of the anionic and cationic species is consistent with a negative charge on the plant surface.

Miller, C.W. and F.O. Hoffman. 1983. "An Examination of the Environmental Half-Time for Radionuclides Deposited on Vegetation." *Health Physics*. 45 (3): 731 to 744.

This document is the source of the equation used to calculate kp:

kp = $(\ln 2 / t_{1/2}) \cdot 365$ days/year
$t_{1/2}$ = half-time (days)

The study reports half-time values ranging from 2.8 to 34 days for a variety of contaminants on herbaceous vegetation. These half-time values result in calculate *kp* values from 7.44 to 90.36 yr^{-1}.

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units*. January.

Shor, R.W., C.F. Baes, and R.D. Sharp. 1982. *Agricultural Production in the United States by County: A Compilation of Information from the 1974 Census of Agriculture for Use in Terrestrial Food-Chain Transport and Assessment Models.* Oak Ridge National Laboratory Publication. ORNL-5786.

This document is the source of the equation used to calculate *Yp*, as cited by U.S. EPA (1994b). Baes, Sharp, Sjoreen, and Shor (1984) also presents and discusses this equation.

Taiz, L., and E. Geiger. 1991. *Plant Physiology*. Benjamin/Cammius Publishing Co. Redwood City, California. 559 pp.

U.S. EPA. 1990. *Interim Final Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Environmental Criteria and Assessment Office. Office of Research and Development. EPA 600/6-90/003. January.

This is one of the source documents for the equation, and also states that the best estimate of *Yp* (yield or standing crop biomass) is productivity, as defined under Shor, Baes, and Sharp (1982).

U.S. EPA. 1993. *Review Draft Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions.* Office of Health and Environmental Assessment. Office of Research and Development. EPA/600/AP-93/003. November.

U.S. EPA. 1994a. *Estimating Exposure to Dioxin-Like Compounds. Volume III: Site-Specific Assessment Procedures. Review Draft.* Office of Research and Development. Washington, D.C. EPA/600/6-88/005Cc. June.

U.S. EPA. 1994b. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. Office of Emergency and Remedial Response. Office of Solid Waste. December 14.

U.S. EPA. 1995. *Review Draft Development of Human Health-Based and Ecologically-Based Exit Criteria for the Hazardous Waste Identification Project*. Volumes I and II. Office of Solid Waste. March 3.

TABLE B-3-2

PLANT CONCENTRATION DUE TO AIR-TO-PLANT TRANSFER (TERRESTRIAL PLANT EQUATIONS)

Description

This equation calculates the COPC concentration in plants, resulting from uptake of vapor phase COPCs by plants through their foliage.

The limitations and uncertainty associated with calculating this value include the following:

(1) The algorithm used to calculate values for the variable F_v assumes a default value for the parameter S_T (Whitby's average surface area of particulates [aerosols]) of background plus local sources, rather than an S_T value for urban sources. If a specific site is located in an urban area, the use of the latter S_T value may be more appropriate. The S_T value for urban sources is about one order of magnitude greater than that for background plus local sources and would result in a lower F_v value; however, the F_v value is likely to be only a few percent lower.

As highlighted by uncertainties described above, *Pv* is most significantly affected by the value calculated for *Bv*.

Equation

$$Pv = Q \cdot F_v \cdot 0.12 \cdot \frac{Cyv \cdot Bv}{\rho_a}$$

For mercury modeling

$$Pv_{Mercury} = (0.48 Q_{TotalMercury}) \cdot F_{v_{Hg^{2+}}} \cdot 0.12 \cdot \frac{Cyv \cdot Bv_{Hg^{2+}}}{\rho_a}$$

In calculating *Pv* for mercury comounds,
Pv(Mercury) is calculated as shown above using the
total mercury emission rate (*Q*) measured at the stack and F_v for mercuric chloride (F_v = 0.85). As presented below, the calculated *Pv(Mercury)* value is apportioned into the divalent mercury (Hg^{2+}) and methyl mercury (MHg) forms based on a 78% Hg^{2+} and 22% MHg speciation split in plants (see Chapter 2).

Pv (Hg^{2+}) = 0.78 *Pv(Mercury)*
Pv (MHg) = 0.22 *Pv(Mercury)*

After calculating species specific *Pv* values, divalent and methyl mercury should continue to be modeled throughout Appendix B equations as individual COPCs.

Variable	Description	Units	Value
Pv	Plant concentration due to air-to-plant transfer	mg/kg WW (equivalent to μg/g)	

TABLE B-3-2

PLANT CONCENTRATION DUE TO AIR-TO-PLANT TRANSFER (TERRESTRIAL PLANT EQUATIONS)

Variable	Description	Units	Value
Q	COPC-specific emission rate	g/s	**Varies (site-specific)** This variable is COPC- and site-specific (see Chapters 2 and 3). Uncertainties associated with this variable are site-specific.
F_v	Fraction of COPC air concentration in vapor phase	unitless	**0 to 1 (see Appendix A-2)** This variable is COPC-specific and should be determined from the COPC tables in Appendix A-2. Uncertainties associated with this variable include the following: (1) Calculation is based on an assumption of a default S_T value for background plus local sources, rather than an S_T value for urban sources. If a specific site is located in an urban area, the use of the latter S_T value may be more appropriate. Specifically, the S_T value for urban sources is about one order of magnitude greater than that for background plus local sources and would result in a lower calculated F_v value; however, the F_v value is likely to be only a few percent lower. (2) According to Bidleman (1988), the equation used to calculate F_v assumes that the variable *c* is constant for all chemicals; however, the value of *c* depends on the chemical (sorbate) molecular weight, the surface concentration for monolayer coverage, and the difference between the heat of desorption from the particle surface and the heat of vaporization of the liquid-phase sorbate. To the extent that site- or COPC-specific conditions may cause the value of *c* to vary, uncertainty is introduced if a constant value of *c* is used to calculate F_v.
Cyv	Unitized yearly air concentration from vapor phase	µg-s/g-m^3	**Varies (modeled)** This variable is COPC- and site-specific, and is determined by air dispersion modeling (see Chapter 3). Uncertainties associated with this variable are site-specific.
Bv	Air-to-plant biotransfer factor	unitless (μg/g plant tissue DW) / (μg/g air)	**Varies (see Appendix C)** This variable is COPC-specific and should be determined from the tables in Appendix C. Uncertainties associated with this variable include the following: (1) The studies that formed the basis of the algorithm used to estimate *Bv* values were conducted on azalea leaves and grasses, and may not accurately represent *Bv* for all forage species of plants.

TABLE B-3-2

PLANT CONCENTRATION DUE TO AIR-TO-PLANT TRANSFER
(TERRESTRIAL PLANT EQUATIONS)

Variable	Description	Units	Value
0.12	Dry weight to wet weight conversion factor	unitless	**0.12** U.S. EPA OSW recommends using the value of 0.12. This default value is based on the average rounded value from the range of 80 to 95 percent water content in herbaceous plants and nonwoody plant parts (Taiz et al. 1991). The following uncertainty is associated with this variable: (1) The plant species considered in determining the default value may be different from plant varieties actually present at a site.
ρ_a	Density of air	g/m^3	**0.0012** U.S. EPA OSW recommends the use of this value based on Weast (1980). This reference indicates that air density varies with temperature. U.S. EPA (1990) recommended this same value but states that it was based on a temperature of 25°C; no reference was provided. U.S. EPA (1994b) and NC DEHNR (1997) recommend this same value but state that it was calculated at standard conditions of 20°C and 1 atm. Both documents cite Weast (1981). There is no significant uncertainty associated with this variable.

TABLE B-3-2

PLANT CONCENTRATION DUE TO AIR-TO-PLANT TRANSFER (TERRESTRIAL PLANT EQUATIONS)

REFERENCES AND DISCUSSION

Bacci E., D. Calamari, C. Gaggi, and M. Vighi. 1990. "Bioconcentration of Organic Chemical Vapors in Plant Leaves: Experimental Measurements and Correlation." *Environmental Science and Technology*. Volume 24. Number 6. Pages 885-889.

This is the source of the equation to adjust B_{vol}, based on volume/volume basis, to *Bv* on a mass/mass basis—see Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992) below.

Bacci E., M. Cerejeira, C. Gaggi, G. Chemello, D. Calamari, and M. Vighi. 1992. "Chlorinated Dioxins: Volatilization from Soils and Bioconcentration in Plant Leaves." *Bulletin of Environmental Contamination and Toxicology*. Volume 48. Pages 401-408.

This is the source of the algorithm based on a study of 14 organic compounds, including 1,2,3,4-TCDD, used to calculate the air-to-plant biotransfer factor (*Bv*):

$$\log B_{vol} = 1.065 \log K_{ow} - \log \left(\frac{H}{R.T_a}\right) - 1.654$$

where:

B_{vol}	=	Volumetric air-to-plant bio transfer factor ([μg/L wet leaf]/[μg/L air])
K_{ow}	=	Octanol-water partition coefficient (dimensionless)
H	=	Henry's Law Constant (atm-m^3/ mol)
R	=	Ideal gas constant, 8.2 x 10^{-5} atm-m^3/mol-deg K
T_a	=	Ambient air temperature, 298.1 K (25°C)

This volumetric transfer factor can be transformed to a mass-based transfer factor by using the following equation (Bacci, Calamari, Gaggi, and Vighi 1990):

$$Bv = \frac{\rho_a \cdot B_{vol}}{(1 - f_{wc}) \cdot \rho_{forage}}$$

where:

Bv	=	mass-based air-to-plant biotransfer factor ([μg/g DW plant]/[μg/g air])
B_{vol}	=	volumetric air-to-plant biotransfer factor ([μg/L wet leaf]/[μg/L air])
ρ_a	=	density of air, 1.19 g/L (Weast 1986)
ρ_{forage}	=	density of forage, 770 g/L (McCrady and Maggard, 1993)
f_{wc}	=	fraction of forage that is water, 0.85 (McCrady and Maggard, 1993)

Bidleman, T.F. 1988. "Atmospheric Processes." *Environmental Science and Technology*. Volume 22. Number 4. Pages 361-367.

This is the reference for the statement that the equation used to calculate the fraction of air concentration in vapor phase (F_v) assumes that the variable *c* (the Junge constant) is constant for all chemicals; however, this reference notes that the value of *c* depends on the chemical (sorbate) molecular weight, the surface concentration for monolayer coverage, and the difference between the heat of desorption from the particle surface and the heat of vaporization of the liquid-phase sorbate.

This document is also cited by U.S. EPA (1994b) and NC DEHNR (1997) for calculating the variable F_v.

NC DEHNR. 1997. *NC DEHNR Protocol for Performing Indirect Exposure Risk Assessments for Hazardous Waste Combustion Units*. January.

Taiz, L., and E. Geiger. 1991. *Plant Physiology*. Benjamin/Cammius Publishing Co. Redwood City, California. 559 pp.

U.S. EPA. 1990. *Interim Final Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. Environmental Criteria and Assessment Office. Office of Research and Development. EPA-600-90-003. January.

This document is a source of air density values.

U.S. EPA. 1993. *Review Draft Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. Office of Health and Environmental Assessment. Office of Research and Development. EPA-600-AP-93-003. November 10.

Based on attempts to model background concentrations of dioxin-like compounds in beef on the basis of known air concentrations, this document recommends reducing, by a factor of 10, *Bv* values calculated by using the Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992) algorithm The use of this factor "made predictions [of beef concentrations] come in line with observations."

U.S. EPA. 1994a. *Estimating Exposure to Dioxin-Like Compounds. Volume II: Properties, Sources, Occurrence, and Background Exposures. Review Draft.* Office of Research and Development. Washington, DC. EPA/600/6-88/005Cb. June.

U.S. EPA. 1994b. *Revised Draft Guidance for Performing Screening Level Risk Analyses at Combustion Facilities Burning Hazardous Wastes. Attachment C, Draft Exposure Assessment Guidance for RCRA Hazardous Waste Combustion Facilities*. Office of Emergency and Remedial Response. Office of Solid Waste. December 14.

This is one of the source documents for Equation B-2-8. This document also presents a range (0.27 to 1) of F_v values for organic COPCs, based on the work of Bidleman (1988); F_v for all inorganics is set equal to zero.

Weast, R.C. 1981. *Handbook of Chemistry and Physics*. 62nd Edition. Cleveland, Ohio. CRC Press.

This document is a reference for air density values.

Weast, R.C. 1986. *Handbook of Chemistry and Physics*. 66th Edition. Cleveland, Ohio. CRC Press.

This document is a reference for air density values, and is an update of Weast (1981).

Wipf, H.K., E. Homberger, N. Neuner, U.B. Ranalder, W. Vetter, and J.P. Vuilleumier. 1982. "TCDD Levels in Soil and Plant Samples from the Seveso Area." *In: Chlorinated Dioxins and Related Compounds: Impact on the Environment*. Eds. Hutzinger, O. and others. Pergamon, NY.

TABLE B-3-3

PLANT CONCENTRATION DUE TO ROOT UPTAKE
(TERRESTRIAL PLANT EQUATIONS)

Description

This equation calculates the COPC concentration in plants, resulting from direct uptake of COPCs from soil through plant roots.

The limitations and uncertainty associated with calculating this value include the following:

(1) The availability of site-specific information, such as meteorological data, may affect the accuracy of *Cs* estimates.
(2) Estimated COPC-specific soil-to-plant bioconcentration factors (BCF_r) may not reflect site-specific conditions.

Equation

$$Pr = Cs \cdot BCF_r \cdot 0.12$$

For mercury modeling:

$$Pr_{(Hg^{2+})} = Cs_{(Hg^{2+})} \cdot BCF_{r\,(Hg^{2+})} \cdot 0.12$$

$$Pr_{(MHg)} = Cs_{(MHg)} \cdot BCF_{r\,(MHg)} \cdot 0.12$$

Plant concentration due to root uptake is calculated using the respective *Cs* and BCF_r values for divalent mercury (Hg^{2+}) and methyl mercury (MHg).

Variable	Description	Units	Value
Pr	Plant concentration due to root uptake	mg/kg WW	
Cs	COPC concentration in soil	mg/kg	**Varies (calculated - Table B-1-1)** This value is COPC-and site-specific and should be calculated using the equation in Table B-1-1. Uncertainties associated with this variable are site-specific.

TABLE B-3-3

PLANT CONCENTRATION DUE TO ROOT UPTAKE
(TERRESTRIAL PLANT EQUATIONS)

(Page 2 of 3)

Variable	Description	Units	Value
0.12	Dry weight to wet weight conversion factor	unitless	**0.12** U.S. EPA OSW recommends using the value of 0.12. This default value is based on the average rounded value from the range of 80 to 95 percent water content in herbaceous plants and nonwoody plant parts (Taiz et al. 1991). The following uncertainty is associated with this variable: (1) The plant species considered in determining the default value may be different from plant varieties actually present at a site.
BCF_r	Plant-soil biotransfer factor	unitless [(mg/kg plant DW)/(mg/ kg soil)]	**Varies (see Appendix C)** This variable is COPC-specific. Discussion of this variable and COPC-specific values are presented in Appendix C. Uncertainties associated with this variable include the following: (1) Estimates of BCF_r for some inorganic COPCs, based on plant uptake response slope factors, may be more accurate than those based on BCF values from Baes, Sharp, Sjoreen, and Shor (1984). (2) U.S. EPA OSW recommends that uptake of organic COPCs from soil and transport of the COPCs to the aboveground portions of the plant be calculated on the basis of a regression equation developed in a study of the uptake of 29 organic compounds. This regression equation, developed by Travis and Arms (1988), may not accurately represent the behavior of all organic COPCs under site-specific conditions.

TABLE B-3-3

PLANT CONCENTRATION DUE TO ROOT UPTAKE
(TERRESTRIAL PLANT EQUATIONS)

REFERENCES AND DISCUSSION

Baes, C.F., R.D. Sharp, A.L. Sjoreen, and R.W. Shor. 1984. *Review and Analysis of Parameters and Assessing Transport of Environmentally Released Radionuclides through Agriculture.* ORNL-5786. Oak Ridge National Laboratory. Oak Ridge, Tennessee. September.

Taiz, L., and E. Geiger. 1991. *Plant Physiology*. Benjamin/Cammius Publishing Co. Redwood City, California. 559 pp.

Travis, C.C. and A.D. Arms. 1988. "Bioconcentration of Organics in Beef, Milk, and Vegetation." *Environmental Science and Technology*. 22:271 to 274.

Based on paired soil and plant concentration data for 29 organic compounds, this document developed a regression equation relating soil-to-plant BCF to K_{ow};

$$\log BCF_r = 1.588 - 0.578 \log K_{ow}$$

U.S. EPA. 1995. *Review Draft Development of Human Health-Based and Ecologically-Based Exit Criteria for the Hazardous Waste Identification Project*. Volumes I and II. Office of Solid Waste. March 3.

This document recommended using the BCFs, *Bv* and *Br*, from Baes, Sharp, Sjoreen, and Shor (1984), for calculating the uptake of inorganics into vegetative growth (stems and leaves) and nonvegetative growth (fruits, seeds, and tubers), respectively.

Although most BCFs used in this document come from Baes, Sharp, Sjoreen, and Shor (1984), values for some inorganics were apparently obtained from plant uptake response slope factors. These uptake response slope factors were calculated from field data, such as metal methodologies, and references used to calculate the uptake response slope factors are not clearly identified.

APPENDIX C

MEDIA-TO-RECEPTOR BIOCONCENTRATION FACTORS (*BCF*s)

Screening Level Ecological Risk Assessment Protocol

August 1999

APPENDIX C

TABLE OF CONTENTS

Section **Page**

APPENDIX C

MEDIA-TO-RECEPTOR *BCF*s

Appendix C provides recommended guidance for determining values for media-to-receptor bioconcentration factors (*BCF*s) based on values reported in the scientific literature, or estimated using physical and chemical properties of the compound. Guidance on use of *BCF* values in the screening level ecological risk assessment is provided in Chapter 5.

Section C-1.0 provides the general guidance recommended to select or estimate *BCF* values. Sections C-1.1 through C-1.7 further discuss determination of *BCF*s for specific media and receptors. References cited in Sections C-1.1 through C-1.7 are located following Section C-1.7.

For the compounds commonly identified in risk assessments for combustion facilities (identified in Chapter 2), *BCF* values have been determined following the guidance in Sections C-1.1 through C-1.7. *BCF* values for these limited number of compounds are included in this appendix in Tables C-1 through C-7 to facilitate the completion of screening ecological risk assessments. However, it is expected that additional compounds may require evaluation on a site specific basis, and in such cases, *BCF* values for these additional compounds could be determined following the same guidance (Sections C-1.1 through C-1.7) used in determination of the *BCF* values reported in this appendix. For reproducibility and to facilitate comparison of new data and values as they become available, all data reviewed in the selection of the *BCF* values provided at the end of this appendix are also included in Tables C-1 through C-7. References cited in Tables C-1 through C-7 (Media-to-Receptor *BCF* Values) are located following Table C-7.

For additional discussion on some of the references and equations cited in Sections C-1.1 through C-1.7, the reader is recommended to review the Human Health Risk Assessment Protocol (HHRAP) (U.S. EPA 1998) (see Appendix A-3), and the source documents cited in the reference section of this appendix.

C-1.0 GENERAL GUIDANCE

This section summarizes the recommended general guidance for determining compound-specific *BCF* values (media-to-receptors) provided in Tables C-1 through C-7. As a preference, *BCF* values were selected from empirical field and/or laboratory data generated from reviewed studies that are published in the scientific literature. Information used from these studies included calculated *BCF* values, as well as, collocated media and organism concentration data from which *BCF* values could be calculated. If two or more *BCF* values, or two or more sets of collocated data, were available in the published scientific literature, the geometric mean of the values was used.

Field-derived *BCF* values were considered more indicative of the level of bioconcentration occurring in the natural environment than laboratory-derived values. Therefore, when available and appropriate, field-derived *BCF* values were given priority over laboratory-derived values. In some cases, confidence in the methods used to determine or report field-derived *BCF* values was less than for the laboratory-derived values. In those cases, the laboratory-derived values were used for the recommended *BCF* values.

When neither field or laboratory data were available for a specific compound, data from a potential surrogate compound were evaluated. The appropriateness of the surrogate was determined by comparing the structures of the two compounds. Where an appropriate surrogate was not identified, a regression equation based on the compound's log K_{ow} value was used to calculate the recommended *BCF* value.

With the exception of the air-to-plant biotransfer factors (*Bv*), recommended *BCF* values provided in the tables at the end of this appendix are based on wet tissue weight and dry media weight (except for water). As necessary, reported values were converted to these units using the referenced tissue or media wet weight percentages. The conversion factors, equations, and references for these conversions are discussed in Sections C-1.1 through C-1.7 where appropriate, and are presented at the end of each table (Tables C-1 through C-7).

C-1.1 SOIL-TO-SOIL INVERTEBRATE BIOCONCENTRATION FACTORS

Soil-to-soil invertebrate *BCF* values (see Table C-1) were developed mainly from data for earthworms. Measured experimental results were primarily in the form of ratios of compound concentrations in a earthworm and the compound concentrations in the soil in which the earthworm was exposed. As necessary, values were converted to wet tissue and dry media weight assuming a moisture content (by mass) of 83.3 percent for earthworms and 20 percent for soil (Pietz et al. 1984).

Organics For organic compounds with no field or laboratory data available, recommended *BCF* values were estimated using the following regression equation**:**

$$\log BCF = 0.819 \log K_{ow} - 1.146 \qquad \text{Equation C-1-1}$$

- Southworth, G.R., J.J. Beauchamp, and P.K. Schmieder. 1978. "Bioaccumulation Potential of Polycyclic Aromatic Hydrocarbons in *Daphnia Pulex." Water Research.* Volume 12. Pages 973-977.

Inorganics For inorganic compounds with no field or laboratory data available, the recommended *BCF* value is equal to the arithmetic average of the available *BCF* values for other inorganics as specified in Table C-1.

C-1.2 SOIL-TO-PLANT AND SEDIMENT-TO-PLANT BIOCONCENTRATION FACTORS

Soil-to-plant *BCF* values (see Table C-2) account for plant uptake of compounds from soil. Data for a variety of plants and food crops were used to determine recommended *BCF* values.

Organics For all organics (including PCDDs and PCDFs) with no available field or laboratory data, the following regression equation was used to calculate recommended values:

$$\log BCF = 1.588 - 0.578 \log K_{ow} \qquad \text{Equation C-1-2}$$

- Travis, C.C. and A.D. Arms. 1988. "Bioconcentration of Organics in Beef, Milk, and Vegetation." *Environmental Science and Technology.* 22:271-274.

Inorganics For most metals, *BCF* values were based on empirical data reported in the following:

- Baes, C.F., R.D. Sharp, A.L. Sjoreen, and R.W. Shor. 1984. "Review and Analysis of Parameters and Assessing Transport of Environmentally Released Radionuclides Through Agriculture." Oak Ridge National Laboratory, Oak Ridge, Tennessee.

The scientific literature also was searched to identify studies. Although U.S. EPA (1995a) provides values for certain metals calculated on the basis of plant uptake response slope factors, it is unclear how the *BCF*

values were calculated or which sources or references were used. Therefore, values reported in U.S. EPA (1995a) were not used.

C-1.3 WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS

Experimental data for crustaceans, aquatic insects, bivalves, and other aquatic invertebrates were used to determine recommended *BCF* values for water-to-aquatic invertebrate (see Table C-3). Both marine and freshwater exposures were reviewed. As necessary, available results were converted to wet tissue weight assuming that invertebrate moisture content (by mass) is 83.3 percent (Pietz et al. 1984).

Organics Reported field values for organic compounds were assumed to be total compound concentrations in water and, therefore, were converted to dissolved compound concentrations in water using the following equation from U.S. EPA (1995b):

$$BCF \text{ (dissolved)} = (BCF \text{ (total)} / f_{fd}) - 1 \qquad \text{Equation C-1-3}$$

where

BCF (dissolved)	=	*BCF* based on dissolved concentration of compound in water
BCF (total)	=	BCF based on the field derived data for total concentration of compound in water
f_{fd}	=	Fraction of compound that is freely dissolved in the water

and,

f_{fd}	=	$1 / [1 + ((DOC \times K_{ow}) / 10) + (POC \times K_{ow})]$
DOC	=	Dissolved organic carbon, kilograms of organic carbon / liter of water (2.0×10^{-06} Kg/L)
K_{ow}	=	Octanol-water partition coefficient of the compound, as reported in U.S. EPA (1994a)
POC	=	Particulate organic carbon, kilograms of organic carbon / liter of water (7.5×10^{-09} Kg/L)

Laboratory data were assumed to be based on dissolved compound concentrations.

For organic compounds with no field or laboratory data available, *BCF* values were determined from surrogate compounds or calculated using the following regression equation:

$$log\ BCF = 0.819 \times log\ K_{ow} - 1.146 \qquad \text{Equation C-1-4}$$

- Southworth, G.R., J.J. Beauchamp, and P.K. Schmieder. 1978. "Bioaccumulation Potential of Polycyclic Aromatic Hydrocarbons in *Daphnia Pulex.*" *Water Research*. Volume 12. Pages 973-977.

Inorganics For inorganic compounds with no field or laboratory data available, the recommended *BCF* values were estimated as the arithmetic average of the available *BCF* values for other inorganics, as specified in Table C-3.

C-1.4 WATER-TO-ALGAE BIOCONCENTRATION FACTORS

Experimental data for both marine and freshwater algal species were reviewed. As necessary, available results were converted to wet tissue weight assuming that algae moisture content (by mass) is 65.7 percent (Isensee et al. 1973).

Organics For organic compounds with no field or laboratory data available, *BCF* values were calculated using the following regression equation:

$$log\ BCF = 0.819 \times log\ K_{ow} - 1.146 \qquad \text{Equation C-1-5}$$

- Southworth, G.R., J.J. Beauchamp, and P.K. Schmieder. 1978. "Bioaccumulation Potential of Polycyclic Aromatic Hydrocarbons in *Daphnia Pulex.*" *Water Research*. Volume 12. Pages 973-977.

Inorganics For inorganics, available field or laboratory data were evaluated for each compound.

C-1.5 WATER-TO-FISH BIOCONCENTRATION FACTORS

Experimental data for a variety of marine and freshwater fish were used to determine recommended *BCF* values (see Table C-5). As necessary, values were converted to wet tissue weight assuming that fish moisture content (by mass) is 80.0 percent (Holcomb et al. 1976).

For both organic and inorganic compounds, reported field values were considered bioaccumulation factors (*BAF*s) based on contributions of compounds from food sources as well as media. Therefore, field values were converted to *BCF*s based on the trophic level of the test organism using the following equation:

$$BCF = (BAF_{TLn} / FCM_{TLn}) - 1 \qquad \text{Equation C-1-6}$$

where

BAF_{TLn}	=	The reported field bioaccumulation factor for the trophic level "n" of the study species.
FCM_{TLn}	=	The food chain multiplier for the trophic level "n" of the study species.

Organics Reported field values for organic compounds were assumed to be total compound concentrations in water and, therefore, were converted to dissolved compound concentrations in water using the following equation from U.S. EPA (1995b):

$$BAF\ (\text{dissolved}) = (BAF\ (\text{total}) / f_{fd}) - 1 \qquad \text{Equation C-1-7}$$

where

BAF (dissolved)	=	*BAF* based on dissolved concentration of compound in water
BAF (total)	=	*BAF* based on the field derived data for total concentration of compound in water
f_{fd}	=	Fraction of compound that is freely dissolved in the water

and,

f_{fd}	=	1 / [1 + ((DOC x K_{ow}) / 10) + (POC x K_{ow})]
DOC	=	Dissolved organic carbon, Kg of organic carbon / L of water (2.0 x 10^{-06} Kg/L)
K_{ow}	=	Octanol-water partition coefficient of the compound, as reported in U.S. EPA (1994a)
POC	=	Particulate organic carbon, Kg of organic carbon / L of water (7.5 x 10^{-09} Kg/L)

Laboratory data were assumed to be based on dissolved compound concentrations.

For organics for which no field or laboratory data were available, the following regression equation was used to calculate the recommended *BCF* values:

$$log\ BCF = 0.91 \times log\ K_{ow} - 1.975 \times log\ (6.8E\text{-}07 \times K_{ow} + 1.0) - 0.786 \qquad \text{Equation C-1-8}$$

- Bintein, S., J. Devillers, and W. Karcher. 1993. "Nonlinear Dependence of Fish Bioconcentrations on n-Octanol/Water Partition Coefficients." *SAR and QSAR in Environmental Research*. Vol. 1. Pages 29-39.

Inorganics For inorganic compounds with no available field or laboratory data, the recommended *BCF* values were estimated as the arithmetic average of the available *BCF* values reported for other inorganics.

C-1.6 SEDIMENT-TO-BENTHIC INVERTEBRATE BIOCONCENTRATION FACTORS

Experimental data for a variety of benthic infauna, worms, insects, and other invertebrates were used to determine the recommended *BCF* values for sediment-to-benthic invertebrate (see Table C-6). As necessary, values were converted to wet tissue weight assuming that benthic invertebrate moisture content (by mass) is 83.3 percent (Pietz et al. 1984).

Organics For organic compound (including PCDDs and PCDFs) with no available field or laboratory data, the recommended *BCF* values were determined using the following regression equation:

$$log\ BCF = 0.819 \times log\ K_{ow} - 1.146 \qquad \text{Equation C-1-9}$$

- Southworth, G.R., J.J. Beauchamp, and P.K. Schmieder. 1978. "Bioaccumulation Potential of Polycyclic Aromatic Hydrocarbons in *Daphnia Pulex.*" *Water Research*. Volume 12. Pages 973-977.

Inorganics For inorganic compound with no available field or laboratory data, the recommended *BCF* values were estimated as the arithmetic average of the available *BCF* values for other inorganics.

C-1.7 AIR-TO-PLANT BIOCONCENTRATION FACTORS

The air-to-plant bioconcentration (*Bv*) factor (see Table C-7) is defined as the ratio of compound concentrations in exposed aboveground plant parts to the compound concentration in air. Bv values in Table C-7 are reported on dry-weight basis since the plant concentration equations (see Chapter 3) already include a dry-weight to wet-weight conversion factor.

Organics For organics (excluding PCDDs and PCDFs), the air-to-plant bioconcentration factor was calculated using regression equations derived for azalea leaves in the following documents:

- Bacci E., D. Calamari, C. Gaggi, and M. Vighi. 1990. "Bioconcentration of Organic Chemical Vapors in Plant Leaves: Experimental Measurements and Correlation." *Environmental Science and Technology*. Volume 24. Number 6. Pages 885-889.

- Bacci E., M. Cerejeira, C. Gaggi, G. Chemello, D. Calamari, and M. Vighi. 1992. "Chlorinated Dioxins: Volatilization from Soils and Bioconcentration in Plant Leaves." *Bulletin of Environmental Contamination and Toxicology*. Volume 48. Pages 401-408.

Bacci et al. (1992) developed a regression equation using empirical data collected for the uptake of 1,2,3,4-TCDD in azalea leaves and data obtained from Bacci et al. (1990). The bioconcentration factor obtained was included in a series of 14 different organic compounds to develop a correlation equation with K_{ow} and H (defined below). Bacci et al. (1992) derived the following equations:

$$\log B_{vol} = 1.065 \log K_{ow} - \log \left(\frac{H}{RT}\right) - 1.654 \qquad (r = 0.957) \qquad \text{Equation C-1-10}$$

$$Bv = \frac{\rho_{air} \cdot B_{vol}}{(1 - f_{water}) \cdot \rho_{forage}} \qquad \text{Equation C-1-11}$$

where

B_{vol}	=	Volumetric air-to-plant biotransfer factor (fresh-weight basis)
Bv	=	Air-to-plant biotransfer factor (dry-weight basis)
ρ_{air}	=	1.19 g/L (Weast 1986)
ρ_{forage}	=	770 g/L (Macrady and Maggard 1993)
f_{water}	=	0.85 (fraction of forage that is water—Macrady and Maggard [1993])
H	=	Henry's Law constant (atm-m^3/mole)
R	=	Universal gas constant (atm-m^3/mole °K)
T	=	Temperature (25°C, 298°K)

Equations C-1-10 and C-1-11 are used to calculate *Bv* values (see Table C-7) using the recommended values of H and K_{ow} provided in Appendix A at a temperature (T) of 25 °C or 298.1 K. The following uncertainty should be noted with use of *Bv* values calculated using these equations:

- For organics (except PCDDs and PCDFs), U.S. EPA (1993) recommended that *Bv* values be reduced by a factor of 10 before use. This was based on the work conducted by U.S. EPA (1993) for U.S. EPA (1994b) as an interim correction factor. Welsch-Pausch, McLachlan, and Umlauf (1995) conducted experiments to determine concentrations of PCDDs and PCDFs in air and resulting biotransfer to welsh ray grass. This was documented in the following:

  - Welsch-Pausch, K.M. McLachlan, and G. Umlauf. 1995. "Determination of the Principal Pathways of Polychlorinated Dibenzo-p-dioxins and Dibenzofurans to Lolium Multiflorum (Welsh Ray Grass)". *Environmental Science and Technology*. 29: 1090-1098.

  A follow-up study based on Welsch-Pausch, McLachlan, and Umlauf (1995) experiments was conducted by Lorber (1995) (see discussion below for PCDDs and PCDFs). In a following publication, Lorber (1997) concluded that the Bacci factor reduced by a factor of 100 was close in line with observations made by him through various studies, including the Welsch-Pausch, McLachlan, and Umlauf (1995) experiments. Therefore, this guidance recommends that *Bv* values be calculated using the Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992) correlation equations and then reduced by a factor of 100 for all organics, excluding PCDDs and PCDFs.

PCDDs and PCDFs For PCDDs and PCDFs, *Bv* values, on a dry weight basis, were obtained from the following:

- Lorber, M., and P. Pinsky. 1999. "An Evaluation of Three Empirical Air-to-Leaf Models for Polychlorinated Dibenzo-p-Dioxins and Dibenzofurans." National Center for Environmental Assessment (NCEA). U. S. EPA, 401 M St. SW, Washington, DC. *Accepted for Publication in Chemosphere*.

U.S. EPA (1993) stated that, for dioxin-like compounds, the use of the Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992) equations may overpredict *Bv* values by a factor of 40. This was because the Bacci, Calamari, Gaggi, and Vighi (1990) and Bacci, Cerejeira, Gaggi, Chemello, Calamari, and Vighi (1992) experiments did not take photodegradation effects into account. Therefore, *Bv* values calculated using Equations C-10 and C-11 were recommended to be reduced by a factor of 40 for dioxin-like compounds.

However, according to Lorber (1995), the Bacci algorithm divided by 40 may not be appropriate because (1) the physical and chemical properties of dioxin congeners are generally outside the range of the 14 organic compounds used by Bacci, Calamari, Gaggi, and Vighi (1990), and (2) the factor of 40 derived from one experiment on 2,3,7,8-TCDD may not apply to all dioxin congeners.

Welsch-Pausch, McLachlan, and Umlauf (1995) conducted experiments to obtain data on uptake of PCDDs and PCDFs from air to *Lolium Multiflorum* (Welsh Ray grass). The data includes grass concentrations and air concentrations for dioxin-congener groups, but not the invidual congeners. Lorber (1995) used data from Welsch-Pausch, McLachlan, and Umlauf (1995) to develop an air-to-leaf transfer factor for each dioxin-congener group. *Bv* values developed by Lorber (1995) were about an order of magnitude less than values that would have been calculated using the Bacci, Calamari, Gaggi, and Vighi (1990; 1992) correlation equations. Lorber (1995) speculated that this difference could be attributed to several factors including experimental design, climate, and lipid content of plant species used.

Lorber (1999) conducted an evaluation of three empirical air-to-leaf models for estimating grass concentraions of PCDDs and PCDFs from air concentrations of these compounds described and tested against field data. *Bv* values recommended for PCDDs and PCDFs in this guidance were obtained from the experimentally derived values of Lorber (1999).

Metals For metals, no literature sources were available for *Bv* values. U.S. EPA (1995a) quoted from the following document, that metals were assumed not to experience air to leaf transfer:

- Belcher, G.D., and C.C. Travis. 1989. "Modeling Support for the RURA and Municipal Waste Combustion Projects: Final Report on Sensitivity and Uncertainty Analysis for the Terrestrial Food Chain Model." Interagency Agreement No. 1824-A020-A1. Office of Risk Analysis, Health and Safety Research Division. Oak Ridge National Laboratory. Oak Ridge, Tennessee. October.

Consistent with the above references, *Bv* values for metals (excluding elemental mercury) were assumed to be zero (see Table C-7).

Mercuric Compounds Mercury emissions are assumed to consist of both the elemental and divalent forms. However, only small amounts of elemental mercury is assumed to be deposited (see Chapter 2). Elemental mercury either dissipates into the global cycle or is converted to the divalent form. Methyl mercury is assumed not to exist in the stack emissions or in the air phase. Consistent with various discussions in Chapter 2 concerning mercury, (1) elemental mercury reaching or depositing onto the plant surfaces is negligible, and (2) biotransfer of methyl mercury from air is zero. This is based on assumptions made regarding speciation and fate and transport of mercury from stack emissions. Therefore, the *Bv* value for (1) elemental mercury was assumed to be zero, and (2) methyl mercury was assumed not to be applicable. *Bv* values for mercuric chloride (dry weight basis) were obtained from U.S. EPA (1997).

It should be noted that uptake of mercury from air into the aboveground plant tissue is primarily in the divalent form. A part of the divalent form of mercury is assumed to be converted to the methyl mercury form once in the plant tissue.

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MEDIA-TO-RECEPTOR *BCF* VALUES

Screening Level Ecological Risk Assessment Protocol

August 1999

TABLE C-1

SOIL-TO-SOIL INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC/kg wet tissue) / (mg COPC/kg dry soil)

15Reported Values[a]	References	Experimental Parameters	Species
Dioxins and Furans			
Compound: 2,3,7,8-tetrachlorodibenzo-p-dioxin			Recommended BCF Value: 1.59
The BCF was calculated using the geometric mean of 5 laboratory values for 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) as follows:			
14.5	Martinucci, Crespi, Omodeo, Osella, and Traldi (1983)	20-day exposure	Not specified
9.41 0.64 0.68 0.17	Reinecke and Nash (1984)	20-day exposure	*Allolobaphora caliginosa* *Lumbricus rubellus*
Compound: 1,2,3,7,8-pentachlorodibenzo-p-dioxin			Recommended Value: 1.46
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1.59 x 0.92 =1.46			
Compound: 1,2,3,4,7,8-hexachlorodibenzo-p-dioxin			Recommended Value: 0.49
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1.59 x 0.31 =0.49			
Compound: 1,2,3,6,7,8-hexachlorodibenzo-p-dioxin			Recommended Value: 0.19
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1.59 x 0.12 = 0.19			
Compound: 1,2,3,7,8,9-hexachlorodibenzo-p-dioxin			Recommended Value: 0.22
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1.59 x 0.14 = 0.22			
Compound: 1,2,3,4,6,7,8,-heptachlorodibenzo-p-dioxin			Recommended Value: 0.081
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1.59 x 0.051 = 0.081			
Compound: Octachlorodibenzo-p-dioxin			Recommended Value: 0.019
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1.59 x 0.012 = 0.019			
Compound: 2,3,7,8-tetrachlorodibenzofuran			Recommended BCF Value: 1.27
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1.59 x 0.80 =1.27			
Compound: 1,2,3,7,8-pentachlorodibenzofuran			Recommended BCF Value: 0.32

TABLE C-1

SOIL-TO-SOIL INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC/kg wet tissue) / (mg COPC/kg dry soil)

16Reported Values[a]	References	Experimental Parameters	Species
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1.59 x 0.22 = 0.32			
Compound: 2,3,4,7,8-pentachlorodibenzofuran			Recommended BCF Value: 2.54
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1.59 x 1.6 =2.54			
Compound: 1,2,3,4,7,8-hexachlorodibenzofuran			Recommended BCF Value: 0.121
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1.59 x 0.076 = 0.121			
Compound: 1,2,3,6,7,8-hexachlorodibenzofuran			Recommended BCF Value: 0.30
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1.59 x 0.19 = 0.30			
Compound: 2,3,4,6,7,8-hexachlorodibenzofuran			Recommended BCF Value: 1.07
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1.59 x 0.67 =1.07			
Compound: 1,2,3,7,8,9-hexachlorodibenzofuran			Recommended BCF Value: 1.00
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1.59 x 0.63 = 1.00			
Compound: 1,2,3,4,6,7,8-heptachlorodibenzofuran			Recommended BCF Value: 0.017
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1.59 x 0.011 = 0.017			
Compound: 1,2,3,4,7,8,9-heptachlorodibenzofuran			Recommended BCF Value: 0.62
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1.59 x 0.39 = 0.62			
Compound: Octochlorodibenzofuran			Recommended BCF Value: 0.025
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1.59 x 0.016 = 0.025			
Polynuclear Aromatic Hydrocarbons (PAHs)			
Compound: Benzo(a)pyrene			Recommended BCF Value: 0.07
The BCF was calculated using the geometric mean of 6 laboratory values for benzo(a)pyrene. The values reported in Rhett, Simmers, and Lee (1988) were converted to earthworm wet weight over soil dry weight using a conversion factor of 5.99[a].			

TABLE C-1

SOIL-TO-SOIL INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC/kg wet tissue) / (mg COPC/kg dry soil)

17Reported Values[a]	References	Experimental Parameters	Species
0.12 0.14 0.05 0.04 0.06 0.06	Rhett, Simmers, and Lee (1988)	28-day exposure	*Eisenia foetida*
Compoound: Benzo(a)anthracene			Recommended BCF Value: 0.03
The BCF was calculated using the geometric mean of 15 values for benzo(a)anthracene. The values reported in Marquenie, Simmers, and Kay (1987) were converted to wet weight over dry weight using a conversion factor of 5.99 [a].			
0.07 0.02 0.08 0.02 0.05 0.07 0.07 0.003 0.07 0.05 0.02 0.01 0.01 0.01 0.09	Marquenie, Simmers, and Kay (1987)	32-day exposure	*Eisenia foetida*
Compound: Benzo(b)fluoranthene			Recommended BCF Value: 0.07
The BCF was calculated using the geometric mean of 6 laboratory values for benzo(b)fluoranthene. The values reported in Rhett, Simmers, and Lee (1988) were converted to wet weight over dry weight using a conversion factor of 5.99 [a].			
0.11 0.16 0.06 0.04 0.06 0.05	Rhett, Simmers, and Lee (1988)	28-day exposure	*Eisenia foetida*
Compound: Benzo(k)fluoranthene			Recommended BCF Value: 0.08
The BCF was calculated using the geometric mean of 15 laboratory values for benzo(k)fluoranthene. The values reported in Marquenie, Simmers, and Kay (1987) were converted to wet weight over dry weight using a conversion factor of 5.99[a].			
0.13 0.15 0.12 0.11 0.07 0.24 0.12 0.02 0.10 0.03 0.07 0.03 0.06 0.04	Marquenie, Simmers, and Kay (1987)	32-day exposure	*Eisenia foetida*

TABLE C-1

SOIL-TO-SOIL INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC/kg wet tissue) / (mg COPC/kg dry soil)

18Reported Values[a]	References	Experimental Parameters	Species
Compound: Chrysene			Recommended BCF Value: 0.04
The BCF was calculated using the geometric mean of 15 laboratory values for chrysene. The values reported in Marquenie, Simmers, and Kay (1987) were converted to wet weight over dry weight using a conversion factor of 5.99 [a].			
0.06 0.03 0.09 0.04 0.09 0.07 0.14 0.007 0.14 0.02 0.04 0.02 0.03 0.01 0.10	Marquenie, Simmers, and Kay (1987)	32-day exposure	*Eisenia foetida*
Compound: Dibenzo(a,h)anthracene			Recommended BCF Value: 0.07
The BCF was calculated using the geometric mean of 15 laboratory values for Dibenz(a,h)anthrcene. The values reported in Marquenie, Simmers, and Kay (1987) were converted to wet weight over dry weight using a conversion factor of 5.99 [a].			
0.18 0.13 0.10 0.06 0.06 0.07 0.04 0.10 0.12 0.05 0.07 0.04 0.04 0.05 0.05	Marquenie, Simmers, and Kay (1987)	32-day exposure	*Eisenia foetida*
Compound: Indeno(1,2,3-cd)pyrene			Recommended BCF Value: 0.08
The BCF was calculated using the geometric mean of 6 laboratory values for indeno(1,2,3-cd)pyrene. The values reported in Rhett, Simmers, and Lee (1988) were converted to wet weight over dry weight using a conversion factor of 5.99[a].			
0.07 0.13 0.08 0.09 0.06 0.05	Rhett, Simmers, and Lee (1988)	28-day exposure	*Eisenia foetida*
Polychlorinated Biphenyls (PCBs)			
Compound: Aroclor 1016			Recommended BCF Value: 1.13

TABLE C-1

SOIL-TO-SOIL INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC/kg wet tissue) / (mg COPC/kg dry soil)

19Reported Values[a]	References	Experimental Parameters	Species
The BCF was calculated using the geometric mean of 7 laboratory values for a mixture of PCB congeners. The values reported in Rhett, Simmers, and Lee (1988) and Kreis, Edwards, Cuendet, and Tarradellas (1987) were converted to wet weight over dry weight using a conversion factor of 5.99 [a].			
1.43 0.81 0.75 1.07 1.17	Rhett, Simmers, and Lee (1988)	28-day exposure	*Eisenia foetida*
1.92 1.16	Kreis, Edwards, Cuendet, and Tarradellas (1987)	Chronic exposure	*Nicodrilus* sp.
Compound: Aroclor 1254			Recommended BCF Value: 1.13
The BCF was calculated using the geometric mean of 7 laboratory values for a mixture of PCB congeners. The values reported in Rhett, Simmers, and Lee (1988) and Kreis, Edwards, Cuendet, and Tarradellas (1987) were converted to wet weight over dry weight using a conversion factor of 5.99 [a].			
1.43 0.81 0.75 1.07 1.17	Rhett, Simmers, and Lee (1988)	28-day exposure	*Eisenia foetida*
1.92 1.16	Kreis, Edwards, Cuendet, and Tarradellas (1987)	Chronic exposure	*Nicodrilus* sp.

TABLE C-1

SOIL-TO-SOIL INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC/kg wet tissue) / (mg COPC/kg dry soil)

20Reported Values[a]	References	Experimental Parameters	Species
Nitroaromatics			
Compound: 1,3-Dinitrobenzene			Recommended BCF Value: 1.19
No empirical data were available for 1,3-dinitrobenzene or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 1.491 (U.S. EPA 1994b).			
Compound: 2,4-Dinitrotoluene			Recommended BCF Value: 3.08
No empirical data were available for 2,4-dinitrotoluene or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 1.996 (U.S. EPA 1994b).			
Compound: 2,6-Dinitrotoluene			Recommended BCF Value: 2.50
No empirical data were available for 2,6-dinitrotoluene or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 1.886 (U.S. EPA 1994b).			
Compound: Nitrobenzene			Recommended BCF Value: 2.26
No empirical data were available for nitrobenzene or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 1.833 (U.S. EPA 1994b).			
Compound: Pentachloronitrobenzene			Recommended BCF Value: 451
No empirical data were available for pentachloronitrobenzene or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 4.640 (U.S. EPA 1994b).			
Phthalate Esters			
Compound: Bis(2-ethylhexyl)phthalate			Recommended BCF Value: 1,309
No empirical data were available for bis(2-ethylhexyl)phthalate or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 5.205 (U.S. EPA 1994b).			
Compound: Di(n)octyl phthalate			Recommended BCF Value: 3,128,023
No empirical data were available for di(n)octyl phthalate or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 9.330 (U.S. EPA 1994b).			

TABLE C-1

SOIL-TO-SOIL INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC/kg wet tissue) / (mg COPC/kg dry soil)

21Reported Values[a]	References	Experimental Parameters	Species
Volatile Organic Compounds			
Compound: Acetone			Recommended BCF Value: 0.05
No empirical data were available for acetone or for a structurally-similar surrogate compound.The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder (1978), where log K_{ow} = -0.222 (Karickoff and Long 1995).			
Compound: Acrylonitrile			Recommended BCF Value: 0.11
No empirical data were available for acrylonitrile or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 0.250 (Karickoff and Long 1995).			
Compound: Chloroform			Recommended BCF Value: 2.82
No empirical data were available for chloroform or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 1.949 (U.S. EPA 1994b).			
Compound: Crotonaldehyde			Recommended BCF Value: 0.20
No empirical data were available for crotonaldehyde or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 0.55 (Based on equations developed by Hansch and Leo 1979, calculated in NRC (1981)).			
Compound: 1,4-Dioxane			Recommended BCF Value: 0.04
No empirical data were available for 1,4-dioxane or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = -0.268 (U.S. EPA 1995a).			
Compound: Formaldehyde			Recommended BCF Value: 0.14
No empirical data were available for formaldehyde or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 0.342 (U.S. EPA 1995a).			
Compound: Vinyl chloride			Recommended BCF Value: 0.62
No empirical data were available for vinyl chloride or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 1.146 (U.S. EPA 1994b).			

TABLE C-1

SOIL-TO-SOIL INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC/kg wet tissue) / (mg COPC/kg dry soil)

22Reported Values[a]	References	Experimental Parameters	Species
Other Chlorinated Organics			
Compound: Carbon Tetrachloride			Recommended BCF Value: 12.0
No empirical data were available for carbon tetrachloride or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 2.717 (U.S. EPA 1994b).			
Compound: Hexachlorobenzene			Recommended BCF Value: 2,296
No empirical data were available for hexachlorobenzene or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 5.503 (U.S. EPA 1994b).			
Compound: Hexachlorobutadiene			Recommended BCF Value: 535
No empirical data were available for hexachlorobutadiene or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978) where log K_{ow} = 4.731 (U.S. EPA 1994b).			
Compound: Hexachlorocyclopentadiene			Recommended BCF Value: 745
No empirical data were available for hexachlorocyclopentadiene or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder (1978), where log K_{ow} = 4.907 (U.S. EPA 1994b).			
Compound: Pentachlorobenzene			Recommended BCF Value: 1,050
No empirical data were available for pentachlorobenzene or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder (1978), where log K_{ow} = 5.088 (U.S. EPA 1994b).			
Compound: Pentachlorophenol			Recommended BCF Value: 1,034
No empirical data were available for pentachlorophenol or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder (1978), where log K_{ow} = 5.080 (U.S. EPA 1994b).			
Pesticides			
Compound: 4,4'-DDE			Recommended BCF Value: 1.26
Empirical data for 4,4'-DDE were not available. The BCF was calculated using the geometric mean of 13 laboratory values for 4,4'-DDT. The first six values reported in Gish (1970), Davis (1971), and Beyer and Gish (1980) were converted to wet weight over dry weight using a conversion factor of 5.99[a].			
0.08 0.39 0.29 0.41	Davis (1971)	Chronic exposure	*Lumbricus terrestris*

TABLE C-1

SOIL-TO-SOIL INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC/kg wet tissue) / (mg COPC/kg dry soil)

23Reported Values[a]	References	Experimental Parameters	Species
0.83	Beyer and Gish (1980)	Chronic exposure	*Aporrectodea trapezoides* *Aparrectodea turgida* *Allolobophora chlorotica* *Lumbricus terrestris*
0.85 1.20 2.40 4.60 2.50 1.60	Wheatley and Hardman (1968)	Chronic exposure	Not specified
10.00 14.46	Yadav, Mittad, Agarwal, and Pillai (1981)	Chronic exposure	*Pheretima posthuma*
Compound: Heptachlor			Recommended BCF Value: 1.40
Empirical data for heptachlor were not available. The BCF was calculated using 1 laboratory value for heptachlor epoxide. The value reported in Beyer and Gish (1980) was converted to wet weight over dry weight using a conversion factor of 5.99[a].			
1.40	Beyer and Gish (1980)	Chronic exposure	*Aporrectodea trapezoides* *Aparrectodea turgida* *Allolobophora chlorotica* *Lumbricus terrestris*
Compound: Hexachlorophene			Recommended BCF Value: 106,970
No empirical data were available for hexachlorophene or for a structurally-similar surrogate compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder (1978), where log K_{ow} = 7.540 (Karickoff and Long 1995).			
Inorganics			
Compound: Aluminum			Recommended BCF Value: 0.22
Empirical data for aluminum were not available. The recommended BCF is the arithmetic mean of the recommended values for those inorganics with empirical data available (arsenic, cadmium, chromium, copper, lead, inorganic mercury, nickel, and zinc).			
Compound: Antimony			Recommended BCF Value: 0.22
Empirical data for antimony were not available. The recommended BCF is the arithmetic mean of the recommended values for those inorganics with empirical data available (arsenic, cadmium, chromium, copper, lead, inorganic mercury, nickel, and zinc).			
Compound: Arsenic			Recommended BCF Value: 0.11

TABLE C-1

SOIL-TO-SOIL INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC/kg wet tissue) / (mg COPC/kg dry soil)

24Reported Values[a]	References	Experimental Parameters	Species
The BCF was calculated using the geometric mean of 5 laboratory values for arsenic as listed below. The values reported in Rhett, Simmers, and Lee (1988) were converted to wet weight over dry weight using a conversion factor of 5.99 [a].			
0.14 0.10 0.10 0.17 0.06	Rhett, Simmers, and Lee (1988)	28-day exposure	*Eisenia foetida*
Compound: Barium			Recommended BCF Value: 0.22
Empirical data for barium were not available. The recommended BCF is the arithmetic mean of the recommended values for those inorganics with empirical data available (arsenic, cadmium, chromium, copper, lead, inorganic mercury, nickel, and zinc).			
Compound: Beryllium			Recommended BCF Value: 0.22
Empirical data for beryllium were not available. The recommended BCF is the arithmetic mean of the recommended values for those inorganics with empirical data available (arsenic, cadmium, chromium, copper, lead, inorganic mercury, nickel, and zinc).			
Compound: Cadmium			Recommended BCF Value: 0.96
The BCF was calculated using the geometric mean of 22 laboratory values for cadmium. The values reported in Rhett, Simmers, and Lee (1988) and Simmers, Rhett, and Lee (1983) were converted to wet weight over dry weight using a conversion factor of 5.99[a].			
0.33 0.72 0.25 0.19 3.17 0.55 0.70 0.35	Rhett, Simmers, and Lee (1988)	28-day exposure	*Eisenia foetida*
0.13 0.50 0.29 8.77 1.25 7.86 0.17 6.67 0.11 3.95 8.01 1.50 4.39 2.10	Simmers, Rhett, and Lee (1983)	Chronic exposure	*Allolobophora longa* *A. caliginosa* *A. rosea* *A. chlorotica* *Lumbricus terrestris* *A. lumbricus* *Octolasium* sp.
Compound: Chromium (total)			Recommended BCF Value: 0.01
The BCF was calculated using the geometric mean of 3 laboratory values for chromium. The values reported in Rhett, Simmers, and Lee (1988) were converted to wet weight over dry weight using a conversion factor of 5.99[a].			

TABLE C-1

SOIL-TO-SOIL INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC/kg wet tissue) / (mg COPC/kg dry soil)

25Reported Values[a]	References	Experimental Parameters	Species
0.004 0.004 0.05	Rhett, Simmers, and Lee (1988)	28-day exposure	*Eisenia foetida*
Compound: Copper			Recommended BCF Value: 0.04
The BCF was calculated using the geometric mean of 9 laboratory values for copper. The values reported in Rhett, Simmers, and Lee (1988) were converted to wet weight over dry weight using a conversion factor of 5.99[a].			
0.02 0.03 0.01 0.03 0.20 0.03 0.04 0.04	Rhett, Simmers, and Lee (1988)	28-day exposure	*Eisenia foetida*
0.24	Ma (1987)	Chronic exposure	*Lumbricus rubellus*

TABLE C-1

SOIL-TO-SOIL INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC/kg wet tissue) / (mg COPC/kg dry soil)

26Reported Values[a]	References	Experimental Parameters	Species
Compound: Cyanide (total)			Recommended BCF Value: 1.12
Empirical data for cyanide were not available. The recommended BCF is the arithmetic mean of the recommended values for those inorganics with empirical data available (arsenic, cadmium, chromium, copper, lead, inorganic mercury, methyl mercury, nickel, and zinc).			
Compound: Lead			Recommended BCF Value: 0.03
The BCF was calculated using the geometric mean of 6 laboratory values for lead. The values reported in Rhett, Simmers, and Lee (1988), Ma (1987), and Van Hook (1974) were converted to wet weight over dry weight using a conversion factor of 5.99[a].			
0.02 0.006 0.07	Rhett, Simmers, and Lee (1988)	28-day exposure	*Eisenia foetida*
0.19	Ma (1987)	Chronic exposure	Not specified
0.12	Ma (1982)		Not specified
0.03	Van Hook (1974)	Chronic exposure	*Alabophera* sp. *Lumbricus* sp. *Octolasium* sp.
Compound: Mercuric chloride			Recommended BCF Value: 0.04
The BCF was calculated using the geometric mean of 5 laboratory values for mercuric chloride. The values reported in Rhett, Simmers, and Lee (1988) were converted to wet weight over dry weight using a conversion factor of 5.99[a].			
0.04 0.04 0.06 0.04 0.02	Rhett, Simmers, and Lee (1988)	28-day exposure; tissue concentrations of <0.05 were reported for the first three ratios, however, a concentration of 0.05 was used in order to calculate a conservative BCF value.	*Eisenia foetida*
Compound: Methyl mercury			Recommended BCF Value: 8.50
The BCF was calculated using the geometric mean of 3 laboratory values as presented below. The values reported in Beyer, Cromartie, and Moment (1985) were earthworm wet weight over soil wet weight with 60 percent soil moisture. The soil weight was converted to dry weight to result in the values presented below:			
8.25 8.31 8.95	Beyer, Cromartie, and Moment (1985)	6 to 12-week exposure	*Eisenia foetida*

TABLE C-1

SOIL-TO-SOIL INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC/kg wet tissue) / (mg COPC/kg dry soil)

27Reported Values[a]	References	Experimental Parameters	Species
Compound: Nickel			Recommended BCF Value: 0.02
The BCF was calculated using the geometric mean of 3 laboratory values for nickel. The values reported in Rhett, Simmers, and Lee (1988) were converted to wet weight over dry weight using a conversion factor of 5.99[a].			
0.03 0.01 0.04	Rhett, Simmers, and Lee 1988	28-day exposure	*Eisenia foetida*
Compound: Selenium			Recommended BCF Value: 0.22
Empirical data for selenium were not available. The recommended BCF is the arithmetic mean of the recommended values for those inorganics with empirical data available (arsenic, cadmium, chromium, copper, lead, inorganic mercury, nickel, and zinc).			
Compound: Silver			Recommended BCF Value: 0.22
Empirical data for silver were not available. The recommended BCF is the arithmetic mean of the recommended values for those inorganics with empirical data available (arsenic, cadmium, chromium, copper, lead, inorganic mercury, nickel, and zinc).			
Compound: Thallium			Recommended BCF Value: 0.22
Empirical data for thallium were not available. The recommended BCF is the arithmetic mean of the recommended values for those inorganics with empirical data available (arsenic, cadmium, chromium, copper, lead, inorganic mercury, nickel, and zinc).			

TABLE C-1

SOIL-TO-SOIL INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC/kg wet tissue) / (mg COPC/kg dry soil)

28Reported Values[a]	References	Experimental Parameters	Species
Compound: Zinc			Recommended BCF Value: 0.56
The BCF was calculated using the geometric mean of 5 laboratory values for zinc. The values reported in Rhett, Simmers, and Lee (1988), Ma (1987), and Van Hook (1974) were converted to wet weight over dry weight using a conversion factor of 5.99 [a].			
0.11 0.06 0.58	Rhett, Simmers, and Lee (1988)	28-day exposure	*Eisenia foetida*
10.79	Ma (1987)	Chronic exposure	Not specified
1.28	Van Hook (1974)	Chronic exposure	*Alabophera* sp. *Lumbricus* sp. *Octolasium* sp.

Notes:

(a) The reported values are presented as the amount of COPC in invertebrate tissue divided by the amount of COPC in the soil. If the values reported in the studies were presented as dry tissue weight over dry soil weight, they were converted to wet weight over dry weight by dividing the concentration in dry earthworm tissue weight by 5.99. This conversion factor assumes an earthworm's total weight is 83.3 percent moisture (Pietz et al. 1984).

The conversion factor was calculated as follows:

$$Conversion\ factor = \frac{1.0\ gram\ (g)\ earthworm\ total\ weight}{1.0\ g\ earthworm\ total\ weight - 0.833\ g\ earthworm\ wet\ weight}$$

TABLE C-2

SOIL-TO-PLANT AND SEDIMENT-TO- PLANT BIOCONCENTRATION FACTORS
(mg COPC/kg dry tissue) / (mg COPC/kg dry soil or sediment)

Reported Values	References	Experimental Parameters	Species
Dioxins and Furans			
Compound: 2,3,7,8-Tetrachlorodibenzo-p-dioxin (2,3,7,8-TCDD)			Recommended BCF Value: 0.0056
The BCF for these constituents were calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 6.64 (U.S. EPA 1994a).			
Compound: 1,2,3,7,8-Tetrachlorodibenzo-p-dioxin (1,2,3,7,8-PeCDD)			Recommended BCF Value: 0.0052
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 0.0056 x 0.92 =0.0052			
Compound: 1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin (1,2,3,4,7,8-HxCDD)			Recommended BCF Value: 0.0017
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 0.0056 x0.31 = 0.0017			
Compound: 1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin (1,2,3,6,7,8-HxCDD)			Recommended BCF Value: 0.00067
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 0.0056 x0.12 = 0.00067			
Compound: 1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin (1,2,3,7,8,9-HxCDD)			Recommended BCF Value: 0.00078
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 0.0056 x 0.14 = 0.00078			
Compound: 1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin (1,2,3,4,6,7,8-HpCDD)			Recommended BCF Value: 0.00029
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 0.0056 x0.051 = 0.00029			
Compound: Octachlorodibenzo-p-dioxin (OCDD)			Recommended BCF Value: 0.000067
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 0.0056 x 0.012 = 0.000067			
Compound: 2,3,7,8-Tetrachlorodibenzo-p-furan (2,3,7,8-TCDF)			Recommended BCF Value: 0.0045
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 0.0056 x0.80 = 0.0045			
Compound: 1,2,3,7,8-Pentachlorodibenzo-p-furan (1,2,3,7,8-PeCDF)			Recommended BCF Value: 0.0011
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 0.0056 x0.22 = 0.0011			
Compound: 2,3,4,7,8-Pentachlorodibenzo-p-furan (2,3,4,7,8-PeCDF)			Recommended BCF Value: 0.0090
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 0.0056 x1.6 = 0.0090			

TABLE C-2

SOIL-TO-PLANT AND SEDIMENT-TO- PLANT BIOCONCENTRATION FACTORS
(mg COPC/kg dry tissue) / (mg COPC/kg dry soil or sediment)

Reported Values	References	Experimental Parameters	Species
Compound: 1,2,3,4,7,8-Hexachlorodibenzo-p-furan (1,2,3,4,7,8-HxCDF)			Recommended BCF Value: 0.00043
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 0.0056 x 0.076 = 0.00043			
Compound: 1,2,3,6,7,8-Hexachlorodibenzo-p-furan (1,2,3,6,7,8-HxCDF)			Recommended BCF Value: 0.0011
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 0.0056 x0.19 = 0.0011			
Compound: 2,3,4,6,7,8-Hexachlorodibenzo-p-furan (2,3,4,6,7,8-HxCDF)			Recommended BCF Value: 0.0038
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 0.0056 x0.67 = 0.0038			
Compound: 1,2,3,7,8,9-Hexachlorodibenzo-p-furan (1,2,3,7,8,9-HxCDF)			Recommended BCF Value: 0.0035
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 0.0056 x0.63 = 0.0035			
Compound: 1,2,3,4,6,7,8-Heptachlorodibenzo-p-furan (1,2,3,4,6,7,8-HpCDF)			Recommended BCF Value: 0.000062
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =0.0056 x0.011 = 0.00062			
Compound: 1,2,3,4,7,8,9-Heptachlorodibenzo-p-furan (1,2,3,4,7,8,9-HpCDF)			Recommended BCF Value: 0.0022
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 0.0056 x0.39 = 0.0022			
Compound: Octachlorodibenzo-p-furan (OCDF)			Recommended BCF Value: 0.000090
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 0.0056 x0.016 = 0.000090			
Polynuclear Aromatic Hydrocarbons (PAH)			
Compound: Benzo(a)pyrene			Recommended BCF Value: 0.0
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 6.129 (U.S. EPA 1994b).			
Compound: Benzo(a)anthracene			Recommended BCF Value: 0.0202
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 5.679 (U.S. EPA 1994b).			
Compound Benzo(b)fluoranthene			Recommended BCF Value: 0.0101
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 6.202 (U.S. EPA 1994b).			
Compound: Benzo(k)fluoranthene			Recommended BCF Value: 0.0101

TABLE C-2

SOIL-TO-PLANT AND SEDIMENT-TO- PLANT BIOCONCENTRATION FACTORS
(mg COPC/kg dry tissue) / (mg COPC/kg dry soil or sediment)

Reported Values	References	Experimental Parameters	Species
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 6.2 (Karickhoff and Long 1995).			
Compound: Chrysene			Recommended BCF Value: 0.0187
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 5.739 (U.S. EPA 1994b).			
Compound: Dibenzo(a,h)anthracene			Recommended BCF Value: 0.0064
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 6.547 (U.S. EPA 1994b).			
Compound: Indeno(1,2,3-cd)pyrene			Recommended BCF Value: 0.0039
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 6.915 (U.S. EPA 1994b).			
Polychlorinated Biphenyls (PCBs)			
Compound: Aroclor 1016			Recommended BCF Value: 0.01
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988); using the log K_{ow} for Aroclor 1254, where log K_{ow}= 6.207 (U.S. EPA 1994b).			
Compound: Aroclor 1254			Recommended BCF Value: 0.01
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988); using the log K_{ow} for Aroclor 1254, where log K_{ow}= 6.207 (U.S. EPA 1994b).			
Nitroaromatics			
Compound: 1,3-Dinitrobenzene			Recommended BCF Value: 5.32
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 1.491 (U.S. EPA 1994b).			
Compound: 2,4-Dinitrotoluene			Recommended BCF Value: 2.72
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} =1.996 (U.S. EPA 1994b).			
Compound 2,6-Dinitrotoluene			Recommended BCF Value: 3.15
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 1.886 (U.S. EPA 1994b).			
Compound: Nitrobenzene			Recommended BCF Value: 3.38

TABLE C-2

SOIL-TO-PLANT AND SEDIMENT-TO- PLANT BIOCONCENTRATION FACTORS
(mg COPC/kg dry tissue) / (mg COPC/kg dry soil or sediment)

Reported Values	References	Experimental Parameters	Species
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 1.833 (U.S. EPA 1994b).			
Compound: Pentachloronitrobenzene			Recommended BCF Value: 0.08
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 4.640 (U.S. EPA 1994b).			
Phthalate Esters			
Compound: Bis(2-ethylhexyl)phthalate			Recommended BCF Value: 0.038
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 5.205 (U.S. EPA 1994b).			
Compound: Di(n)octyl phthalate			Recommended BCF Value: 0.000157
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 9.33 (U.S. EPA 1994b).			
Volatile organic compounds			
Compound: Acetone			Recommended BCF Value: 52
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = -0.222 (U.S. EPA 1994c).			
Compound: Acrylonitrile			Recommended BCF Value: 27.77
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 0.250 (Karickhoff and Long 1995).			
Compound: Chloroform			Recommended BCF Value: 2.9
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 1.949 (U.S. EPA 1994b).			
Compound: Crotonaldehyde			Recommended BCF Value: 18.63
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 0.55 (Hansch and Leo 1979).			
Compound: 1,4-Dioxane			Recommended BCF Value: 55.32
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = -0.268 (U.S. EPA 1995c).			
Compound: Formaldehyde			Recommended BCF Value: 24.57
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 0.342 (U.S. EPA (1995c).			
Compound: Vinyl chloride			Recommended BCF Value: 8.43

TABLE C-2

SOIL-TO-PLANT AND SEDIMENT-TO- PLANT BIOCONCENTRATION FACTORS
(mg COPC/kg dry tissue) / (mg COPC/kg dry soil or sediment)

Reported Values	References	Experimental Parameters	Species
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988). where log K_{ow} = 1.146 (U.S. EPA 1994b).			
Other Chlorinated Organics			
Compound: Carbon tetrachloride			Recommended BCF Value: 1.04
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 2.717 (U.S. EPA 1994b).			
Compound: Hexachlorobenzene			Recommended BCF Value: 0.0255
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 5.503 (U.S. EPA 1994b).			
Compound: Hexachlorobutadiene			Recommended BCF Value: 0.0714
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 4.731 (U.S. EPA 1994b).			
Compound: Hexachlorocyclopentadiene			Recommended BCF Value: 0.0565
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 4.907 (U.S. EPA 1994b).			
Compound: Pentachlorobenzene			Recommended BCF Value: 0.044
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 5.088 (U.S. EPA 1994b).			
Compound: Pentachlorophenol			Recommended BCF Value: 0.0449
The BCF was calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988), where log K_{ow} = 5.08 (U.S. EPA 1994b).			
Pesticides			
Compound: 4,4-DDE			Recommended BCF Value: 0.00937
The BCF for these constituents were calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988)., where log K_{ow} = 6.256 (U.S. EPA 1994b).			
Compound: Heptachlor			Recommended BCF Value: 0.0489
The BCF for these constituents were calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988)., where log K_{ow} = 5.015 (U.S. EPA 1994b).			
Compound: Hexachlorophene			Recommended BCF Value: 0.0017

TABLE C-2

SOIL-TO-PLANT AND SEDIMENT-TO- PLANT BIOCONCENTRATION FACTORS
(mg COPC/kg dry tissue) / (mg COPC/kg dry soil or sediment)

Reported Values	References	Experimental Parameters	Species
The BCF for these constituents were calculated using the following regression equation: log BCF = 1.588 - 0.578 x log K_{ow} (Travis and Arms 1988)., where log K_{ow} = 7.54 (Karickhoff and Long 1995).			
Inorganics			
Compound: Aluminum			Recommended BCF Value: 0.004
The BCF for this constituent was based on empirical data reported in Baes, Sharp, Sjoreen and Shor (1984). Experimental parameters were not reported.			
Compound: Antimony			Recommended BCF Value: 0.2
The BCF for this constituent was based on empirical data reported in Baes, Sharp, Sjoreen and Shor (1984). Experimental parameters were not reported.			
Compound: Arsenic			Recommended BCF Value: 0.036
The BCF for this constituent was based on empirical data reported in U.S. EPA (1992c). Experimental parameters were not reported.			
Compound Barium			Recommended BCF Value: 0.15
The BCF for this constituent was based on empirical data reported in Baes, Sharp, Sjoreen and Shor (1984). Experimental parameters were not reported.			
Compound: Beryllium			Recommended BCF Value: 0.01
The BCF for this constituent was based on empirical data reported in Baes, Sharp, Sjoreen and Shor (1984). Experimental parameters were not reported.			
Compound: Cadmium			Recommended BCF Value: 0.364
The BCF for this constituent was based on empirical data reported in U.S. EPA (1992c). Experimental parameters were not reported.			
Compound: Chromium (total)			Recommended BCF Value: 0.0075
The BCF for this constituent was based on empirical data reported in Baes, Sharp, Sjoreen and Shor (1984). Experimental parameters were not reported.			
Compound: Copper			Recommended BCF Value: 0.4
The BCF for this constituent was based on empirical data reported in Baes, Sharp, Sjoreen and Shor (1984). Experimental parameters were not reported.			
Compound: Cyanide (total)			Recommended BCF Value: No data
No empirical or K_{ow} data were available for this constituent.			
Compound: Lead			Recommended BCF Value: 0.045

TABLE C-2

SOIL-TO-PLANT AND SEDIMENT-TO- PLANT BIOCONCENTRATION FACTORS
(mg COPC/kg dry tissue) / (mg COPC/kg dry soil or sediment)

Reported Values	References	Experimental Parameters	Species
The BCF for this constituent was based on empirical data reported in Baes, Sharp, Sjoreen and Shor (1984). Experimental parameters were not reported.			
Compound: Mercuric chloride			Recommended BCF Value: 0.0375
The BCF was calculated using the geometric mean of 3 values for mercuric chloride ($HgCl_2$).			
0.022 0.032 0.075	Cappon (1981)	The values were derived from studies during one growing season using 20 food crop vegetables.	Not specified.
Compound: Methyl mercury			Recommended BCF Value: 0.137
The BCF was calculated using the geometric mean of 3 values for methyl mercury.			
0.062 0.149 0.277	Cappon (1981)	The values were derived from studies during one growing season using 20 food crop vegetables.	Not specified.
Compound: Nickel			Recommended BCF Value: 0.032
The BCF for this constituent was based on empirical data reported in U.S. EPA (1992c). Experimental parameters were not reported.			
Compound: Selenium			Recommended BCF Value: 0.016
The BCF for this constituent was based on empirical data reported in U.S. EPA (1992c). Experimental parameters were not reported.			
Compound: Silver			Recommended BCF Value: 0.4
The BCF for this constituent was based on empirical data reported in Baes, Sharp, Sjoreen and Shor (1984). Experimental parameters were not reported.			
Compound: Thallium			Recommended BCF Value: 0.004
The BCF for this constituent was based on empirical data reported in Baes, Sharp, Sjoreen and Shor (1984). Experimental parameters were not reported.			
Compound: Zinc			Recommended BCF Value: 0.0000000000012
The BCF for this constituent was based on empirical data reported in U.S. EPA (1992c). Experimental parameters were not reported.			

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
Dioxins and Furans			
Compound: 2,3,7,8-Tetrachlorodibenzo(p)dioxin (2,3,7,8-TCDD)			Recommended BCF Value: 1,560
The BCF value was calculated using the geometric mean of 2 values from data reported for 2,3,7,8-tetrachlorodibenzo(p)dioxin (2,3,7,8-TCDD).			
1,762 1,381	Yockim, Isensee, and Jones (1978)	32-day exposure duration	Daphnid; *Heliosoma* sp.
Compound: 1,2,3,7,8-Pentachlorodibenzo(p)dioxin (1,2,3,7,8-PeCDD)			Recommended BCF Value: 1,435
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1,560 x 0.92 =1,435			
Compound: 1,2,3,4,7,8-Hexachlorodibenzo(p)dioxin (1,2,3,4,7,8-HxCDD)			Recommended BCF Value: 483.6
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1,560 x 0.31 =483.6			
Compound: 1,2,3,6,7,8-Hexachlorodibenzo(p)dioxin (1,2,3,6,7,8-HxCDD)			Recommended BCF Value: 187.2
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1,560 x 0.12 =187.2			
Compound: 1,2,3,7,8,9-Hexachlorodibenzo(p)dioxin (1,2,3,7,8,9-HxCDD)			Recommended BCF Value: 218.4
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1,560 x 0.14 = 218.4			
Compound: 1,2,3,4,6,7,8-Heptachlorodibenzo(p)dioxin (1,2,3,4,6,7,8-HpCDD)			Recommended BCF Value: 79.6
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1,560 x 0.051 = 79.6			
Compound: Octachlorodibenzo(p)dioxin (OCDD)			Recommended BCF Value: 18.7
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1,560 x 0.012 = 18.7			
Compound: 2,3,7,8-Tetrachlorodibenzofuran (2,3,7,8-TCDF)			Recommended BCF Value: 1248
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1,560 x 0.80 = 124			
Compound: 1,2,3,7,8-Pentachlorodibenzofuran (1,2,3,7,8-PeCDF)			Recommended BCF Value: 343.2
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1,560 x 0.22 = 343.2			
Compound: 2,3,4,7,8-Pentachlorodibenzofuran (2,3,4,7,8-PeCDF)			Recommended BCF Value: 2,496

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1,560 x 1.6 = 2,496			
Compound: 1,2,3,4,7,8-Hexachlorodibenzofuran (1,2,3,4,7,8-HxCDF)			Recommended BCF Value: 118.6
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1,560 x 0.076 = 118.6			
Compound: 1,2,3,6,7,8-Hexachlorodibenzofuran (1,2,3,6,7,8-HxCDF)			Recommended BCF Value: 296.4
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1,560 x 0.19 = 296.4			
Compound: 2,3,4,6,7,8-Hexachlorodibenzofuran (2,3,4,6,7,8-HxCDF)			Recommended BCF Value: 1,045
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1,560 x 0.67 = 1,045			
Compound: 1,2,3,7,8,9-Hexachlorodibenzofuran (1,2,3,7,8,9-HxCDF)			Recommended BCF Value: 982.8
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1,560 x 0.63 = 982.8			
Compound: 1,2,3,4,6,7,8-Heptachlorodibenzofuran (1,2,3,4,6,7,8-HpCDF)			Recommended BCF Value: 17.2
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1,560 x 0.011 = 17.2			
Compound: 1,2,3,4,7,8,9-Heptachlorodibenzofuran (1,2,3,4,7,8,9-HpCDF)			Recommended BCF Value: 608.4
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1,560 x 0.39 = 608.4			
Compound: Octachlorodibenzofuran (OCDF)			Recommended BCF Value: 25.0
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =1,560 x 0.016 = 25.0			
Polynuclear Aromatic Hydrocarbons (PAHs)			
Compound: Benzo(a)pyrene			Recommended BCF Value: 4,697
The BCF value was calculated using the geometric mean of 6 laboratory values as follows:			
55,000	Eadie, Landrum, and Faust (1982)	Reported as the mean of the measured PAH concentrations in the test species and the sediment	*Pontoporcia hoyi*
12,761	Newsted and Giesy (1987)	24-hour exposure duration	*Daphnia magna*

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
861	Roesijadi, Anderson, and Blaylock (1978)	7-day exposure duration	*Macoma inquinata*
3,000	Lee, Gardner, Anderson, Blaytock, and Barwell-Clarke (1978)	8-day exposure duration. The reported value was calculated by dividing the wet tissue concentration by the medium concentration [(µg/g)/(µg/L)] conversion factor of 1 x 10^3 was applied to the value.	*Crassostrea virginica*
2,745 2,158	Leversee, Landrum, Giesy, and Fannin (1983)	6-hour exposure duration; 0.2 ppm concentrated humic acid added to test medium	*Daphnia magna*
Compound: Benzo(a)anthracene			Recommended BCF Value: 12,299
The BCF value was calculated using the geometric mean of 3 laboratory values as follows:			
18,000	Lee, Gardner, Anderson, Blaytock, and Barwell-Clarke (1978)	8-day exposure duration; The reported value was calculated by dividing the wet tissue concentration by the medium concentration [(µg/g)/(µg/L)] conversion factor of 1 x 10^3 was applied to the value.	*Crassostrea virginica*
10,225	Newsted and Giesy (1987)	24-hour exposure duration	*Daphnia magna*
10,109	Southworth, Beauchamp, and Schmieder (1978)	24-hour exposure duration	*Daphnia pulex*
Compound: Benzo(b)fluoranthene			Recommended BCF Value: 4,697
Laboratory data were not available for this constituent. The BCF for benzo(a)pyrene was used as a surrogate.			
Compound: Benzo(k)fluoranthene			Recommended BCF Value: 13,225
The BCF value was based on one laboratory value as follows:			
13,225	Newsted and Giesy (1987)	24-hour exposure duration	*Daphnia magna*
Compound: Chrysene			Recommended BCF Value: 980
The BCF value was calculated using the geometric mean of 7 laboratory values as follows:			
5,500	Eastmond, Booth, and Lee (1984)	Not reported	*Daphnia magna*

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
248 199 1,809 418	Millea, Corliss, Farragut, and Thompson (1982)	28-day exposure duration; reported values were based on accumulation in the cephalothorax and abdomen at exposures of 1 or 5 µg/L in a cloed seawater system.	*Penaeus duorarum*
6,088	Newsted and Giesy (1987)	24-hour exposure duration	*Daphnia magna*
694	Roesijadi, Anderson, and Blaylock (1978)	7-day exposure duration	*Macoma inquinata*
Compound: Dibenzo(a,h)anthracene			Recommended BCF Value: 710
The BCF value was calculated using the geometric mean of 2 laboratory values as follows:			
652 773	Leversee, Landrum, Giesy, and Fannin (1983)	6-hour exposure duration	*Daphnia magna*
Compound: Indeno(1,2,3-cd)pyrene			Recommended BCF Value: 4,697
Laboratory data were not available for this constituent. The BCF for benzo(a)pyrene was used as a surrogate.			
Polychlorinated Biphenyls (PCBs)			
Compound: Aroclor 1016			Recommended BCF Value: 13,000
The BCF value for Aroclor 1016 was calulated using one laboratory value as follows:			
13,000	Parrish et al. (1974) as cited in EPA (1980b)	84 day exposure Edible portion	*Crassostrea virginica*
Compound: Aroclor 1254			Recommended BCF Value: 5,538
The BCF value for Aroclor 1254 was calulated using the geometric mean 13 laboratory values as follows:			
41,857 6,900 5,679	Rice and White (1987)	Field study	*Sphaerium striatum*

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
750 740 3,800 1,500 6,200 3,500 2,600 2,700	Mayer, Mehrle, and Sanders (1977)	4 to 21-day exposure	*Orconectes nais; Daphnia magna; Gammarus pseudolimnaeus; Palaemontes kadiakensis; Corydalus cornutus; Culex tarsalis; Chaoborus punctipennis*
120,000	Veith, Kuehl, Puglisi, Glass, and Eaton (177)	Field samples	Zooplankton
340,000 in lipid 51,000 dry tissue	Scura and Theilacker (1977)	45 days exposure	*Brachionus plicatilis*
>27,000	Nimmo et al. (1977) as cited in EPA (1980b)	Field data Whole body	Invertebrates
740	Mayer et al. (1977) as cited in EPA (1980b)	21 days exposure	*Pteronarcys dorsata*
1,500	Mayer et al. (1977) as cited in EPA (1980b)	7 days exposre	*Corydalus cornutus*
750	Mayer et al. (1977) as cited in EPA (1980b)	21 days exposure	*Orconectes nais*
373	Mayer et al. (1977) as cited in EPA (1980b)	5 days exposure	*Nereis diversicolor*
140	Duke et al. (1970) as cited in EPA (1980b)	2 day exposure	*Penaeus duorarum*
8,100	Duke et al. (1970) as cited in EPA (1980b)	2 days exposure	*Crassostrea virginica*
236	Courtney and Langston (1978) as cited in EPA (1980b)	5 days exposure	*Arenicola marina*
Nitroaromatics			
Compound: 1,3-Dinitrobenzene			Recommended BCF Value: 13

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
Laboratory data were not available for this constituent. BCF for 2,4-dinitrotoluene was used as a surrogate.			
Compound: 2,4-Dinitrotoluene			Recommended BCF Value: 13
The recommended BCF value is based on one study as follows:			
13	Liu, Bailey, and Pearson (1983)	4-day exposure duration	*Daphnia magna*
Compound: 2,6-Dinitrotoluene			Recommended BCF Value: 13
Laboratory data were not available for this constituent. BCF for 2,4-dinitrotoluene was used as a surrogate.			
Compound: Nitrobenzene			Recommended BCF Value: 13
Laboratory data were not available for this constituent. BCF for 2,4-dinitrotoluene was used as a surrogate.			
Compound: Pentachloronitrobenzene			Recommended BCF Value: 13
Laboratory data were not available for this constituent. BCF for 2,4-dinitrotoluene was used as a surrogate.			
Phthalate Esters			
Compound: Bis(2-ethylhexyl)phthalate			Recommended BCF Value: 318
The BCF value was calculated using the geometric mean of 12 laboratory values as follows:			
2,497	Brown and Thompson (1982)	14 to 28-day exposure duration	*Mytilus edulis*
257	Perez, Davey, Lackie, Morrison, Murphy, Soper, and Winslow (1983)	30-day exposure duration	*Pitar morrhauna*
48 2237	Sanders, Mayer, and Walsh (1973)	14-day exposure duration; The reported value was calculated by dividing the wet tissue concentration by the medium concentration [(µg/g)/(µg/L)], and a conversion factor of 1 x 10^3 was applied to the value. The reported value was also converted from dry weight to wet weight using a conversion factor of 5.99[a].	*Gammarus pseudolimnacus*
1,214 17,473 2,271 24,456	Sodergren (1982)	27-day exposure duration	*Chironomus* sp.; *Sialis* sp.; *Phanorbis corneus*; *Gammarus pulex*

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
11 10 7 17	Wofford, Wilsey, Neff, Giam, and Neff (1981)	24-hour exposure duration	*Crassostrea virginica*; *Penaeus aztecus*
Compound: Di(n)octyl phahalate			Recommended BCF Value: 5,946
The BCF value was calculated using the geometric mean of 2 laboratory values as follows:			
13,600 2,600	Sanborn, Metcalf, Yu, and Lu (1975)	Not reported	*Physia* sp.; *Daphnia* sp.
Volatile Organic Compounds			
Compound: Acetone			Recommended BCF Value: 0.05
Laboratory data were not available for this constituent. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = -0.222 (Karickoff and Long 1995).			
Compound: Acrylonitrile			Recommended BCF Value: 0.11
Laboratory data were not available for this constituent. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where Log K_{ow} = 0.250 (Karickoff and Long 1995).			
Compound: Chloroform			Recommended BCF Value: 2.82
Laboratory data were not available for this constituent. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 1.949 (U.S. EPA 1994b).			
Compound: Crotonaldehyde			Recommended BCF Value: 0.20
Laboratory data were not available for this constituent. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978) where, log K_{ow} = 0.55 (Based on equation developed by Hansch and Leo (1979), as calculated in NRC (1981)).			
Compound: 1,4-Dioxane			Recommended BCF Value: 0.043
Laboratory data were not available for this constituent. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978) where, log K_{ow} = -0.268 (U.S. EPA 1995a).			
Compound: Formaldehyde			Recommended BCF Value: 0.14
Laboratory data were not available for this constituent. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978) where, log K_{ow} = 0.342 (U.S. EPA 1995a).			

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
Compound: Vinyl chloride			Recommended BCF Value: 0.62
Laboratory data were not available for this constituent.The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978) where, log K_{ow} = 1.146 (U.S. EPA 1994b).			
Other Chlorinated Organics			
Compound: Carbon tetrachloride			Recommended BCF Value: 12
Laboratory data were not available for this constituent. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978) where, log K_{ow} = 2.717 (U.S. EPA 1994b).			
Compound: Hexachlorobenzene			Recommended BCF Value: 2,595
The BCF value was calculated using the geometric mean of 16 laboratory values as follows:			
215,331 8,051 11,064	Baturo and Lagadic (1996)	48 to 120-hour exposure duration	*Lymnaea palustris*
1,360 770 1,510 940 1,630 1,030	Isensee, Holden, Woolson, and Jones (1976)	31-day exposure duration	*Heliosoma* sp.*; Daphnia magna*
287 1,247	Metcalf, Kapoor, Lu, Schuth, and Sherman (1973)	1 to 33-day exposure duration	*Daphnia magna; Physa* sp.
17,140 21,820 5,000	Nebeker, Griffis, Wise, Hopkins, and Barbitta (1989)	28-day exposure duration	*Oligochaete*
24,000	Oliver (1987)	79-day exposure duration	*Oligochaete*
5.5	Schauerte, Lay, Klein, and Korte (1982)	4 to 6-week exposure duration	*Dytiscus marginalis*
Compound: Hexachlorobutadiene			Recommended BCF Value: 10.5
The BCF value was based on four laboratory values from one study as follows:			

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
6.27 45.4 11.1 3.86	Laseter, Bartell, Laska, Holmquist, Condie, Brown, and Evans (1976)	10-day exposure duration	*Procambarus clarki*
Compound: Hexachlorocyclopentadiene			Recommended BCF Value: 1,232
The BCF value was calculated using the geometric mean of 2 laboratory values as follows:			
929 1,634	Lu, Metcalf, Hirwe, and Williams (1975)	Not reported	*Physa* sp. *Culex* sp.
Compound: Pentachlorobenzene			Recommended BCF Value: 2,595
Laboratory data were not available for this constituent. The BCF for hexachlorobenzene was used as a surrogate.			
Compound: Pentachlorophenol			Recommended BCF Value: 52
The BCF value was calculated using the geometric mean of 13 laboratory values as follows:			
145 342	Makela and Oikari (1990)	1-day exposure duration	*Anodonta anatina*
165	Lu and Metcalf (1975)	1-day exposure duration	*Daphnia magna*
81 461	Makela, Petanen, Kukkonen, and Oikari (1991)	Multiple exposure durations	*Anodonta anatina*
80 61 121 85	Makela and Oikari (1995)	2 to 36-week exposure duration	*Anodonta anatina*; *Pseudanodonta complanta*
42 0.26 72 1.7	Schimmel, Patrick, and Faas (1978)	28-day exposure duration	*Crassostrea virginica*; *Penaeus aztecus*; *Palaemonetes pugio*
Pesticides			
Compound: 4,4'-DDE			Recommended BCF Value: 11,930
The recommended BCF value was calculated using the geometric mean of 14 field values[(b)] (Reich, Perkins, and Cutter 1986).			

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
19,400 4,421 207,070 8,782 67,641 2,374 5,099 2,197 8,344 46,953 15,369 35,373 4,983 3,972	Reich, Perkins, and Cutter (1986)	Field samples.	*Tubificidae; Chironomidae; Corixidae*
36,342 39,390	Metcalf, Sanborn, Lu, and Nye (1975)	33-day exposure duration	*Physa* sp.; *Culex pipiens quinquefasciatus*
28,600 1310 63,500 51,600 36,400	Hamelink, Waybrant, and Yant (1977)	Not reported	Zooplankton
19,528 5,024	Metcalf, Sangha, and Kapoor (1971)	33-day exposure duration; The value reported in Hamelink and Waybrant (1976) was converted to wet weight over dry weight using a conversion factor was 5.99[a].	*Physa* sp.; *Culex pipiens quinquefasciatus*
19,529	Metcalf, Kapoor, Lu, Schuth, and Sherman (1973)	33-day exposure duration	*Physa* sp.
Compound: Heptachlor			Recommended BCF Value: 3,807
The BCF value was calculated using the geometric mean of 4 laboratory values as follows:			
37,153 31,403	Lu, Metcalf, Plummer, and Mandel (1975)	Not reported	*Physa* sp. *Culex* sp.
300 600	Schimmel, Patrick, and Forester (1976)	96 hour exposure duration	*Penaeus duorarum*
Compound: Hexachloropehene			Recommended BCF Value: 970
The BCF value was based on one study as follows:			
970	Sanborn (1974)	Not reported	*Physa* sp.
Inorganics			
Compound: Aluminum			Recommended BCF Value: 4,066

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
Laboratory data were not available for this constituent. The recommended BCF is the arithmetic mean of the recommended values for 14 inorganics with laboratory data available (antimony, arsenic, barium, beryllium, cadmium, chromium, copper, lead, mercury, nickel, selenium, silver, thallium, and zinc).			
Compound: Antimony			Recommended BCF Value: 7
The BCF value was calculated using the geometric means of 2 laboratory values as follows:			
10	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Freshwater and marine invertebrates
Compound: Arsenic			Recommended BCF Value: 73
The BCF value was calculated using the geometric mean of 5 laboratory values as follows:			
33 50 45 219 131	Spehar, Fiandt, Anderson, and DeFoe (1980)	21 to 28-day exposure duration	*Pteronarcys dorsata*; *Daphnia magna*
Compound: Barium			Recommended BCF Value: 200
The BCF was based on one study as follows:			
200	Thompson, Burton, Quinn and Ng (1972)	Not reported	Freshwater invertebrate
Compound: Beryllium			Recommended BCF Value: 45
The BCF value was calculated using the geometric mean of 2 laboratory values as follows:			
10 200	Thompson, Burton, Quinn and Ng (1972)	Not reported	Freshwater invertebrate
Compound: Cadmium			Recommended BCF Value: 3,461
The BCF value was calculated using the geometric mean of 8 field values as follows:			
238 549 894 3,577 11,383 15,936 9,897 27,427	Saiki, Castleberry, May, Martin, and Bullard (1995)	Field samples.	*Chironomidea; Ephermeroptera*

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
1,490 2,460 720	Eisler, Zaroogian, and Hennekey (1972)	3-week exposure duration	*Crassostrea virginica*; *Aquipecten irradians*; *Homarus americanus*
165	George and Coombs (1977)	28-day exposure duration	*Mytilus edulis*
1,359 137 2,939 217 615 1,850 573 1,530 1,082 781 775 553	Giesy, Kanio, Boling, Knight, Mashburn, and Clarkin (1977)	52-week exposure duration; the reported value was calculated by dividing the dry tissue concentration by the medium concentration [(µg/g)/(µg/L)] conversion factor of 1 x 10^3 was applied to the value. A conversion factor or 5.99[(a)] was used to convert dry weight to wet weight.	*Ceratopogonidae; Chironomidae;* Beetle*; Anisotptera; Zygoptera; Ephemeroptera*
1,840	Gillespie, Reisine, and Massaro (1977)	8-day exposure duration; the reported value was calculated by dividing the dry tissue concentration by the medium concentration [(ppm)/(ppb)] and a conversion factor of 1 x 10^3 was applied to the value.	*Orconectes propinquos propinquos*
3,770 1,752	Graney, Cherry, and Cairns (1983)	28-day exposure duration	*Corbicula fluminea*
1.86 6.88 7.18	Jennings and Rainbow (1979)	40-day exposure duration; the reported value was calculated by dividing the dry tissue concentration by the medium concentration [(mg/g)/(ppm)] conversion factor of 1 x 10^3 was applied to the value. A conversion factor or 5.99[(a)] was used to convert dry weight to wet weight.	*Carcinus maenas*
660 3400	Klockner (1979)	64-day exposure duration	*Ophryothochadiadema* sp.
48 33 57 34 55 23	Nimmo, Lightner, and Bahner (1977)	28 to 30-day exposure duration	*Penaeus duorarum*
1,023 17.7 1,477 17.5 2,412 30 3,406 28.7 37.2	Pesch and Stewart (1980)	42-day exposure duration; the values reported in Pesch and Stewart (1980) were converted to wet weight using a conversion factor of 5.99[(a)].	*Argopecten irradians*; *Palaemonetes pugio*

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
57 301 341 167	Phillips (1976)	35-day exposure duration; the reported value was calculated by dividing the wet tissue concentration by the medium concentration [(µg/g)/(µg/L)] conversion factor of 1 x 10^3 was applied to the value.	*Mytilus edulis*
160	Pringle, Hissong, Katz, and Mulawka (1968)	70-day exposure duration	*Mya arenaria*
3,500	Sundelin (1983)	66-week exposure duration	*Pontoporeia affinis*
123 89 93 67 48 115	Theede, Scholz, and Fischer (1979)	7 and 10-day exposure duration; the reported value was calculated by dividing the dry tissue concentration by the medium concentration [(µg/g)/(µg/L)] conversion factor of 1 x 10^3 was applied to the value. A conversion factor or 5.99[a] was used to convert dry weight to wet weight.	*Laomedea loveni*
2,150 13,600	Zaroogian and Cheer (1976)	40-week exposure	*Crassostrea virginica*
Compound: Chromium (total)			Recommended BCF Value: 3,000
The BCF value was based on 1 field value as follows:			
3,000	Namminga and Wilhm (1977)	Field samples.	*Chironomidae*
1,900	NAS (1974)	Not reported	Zooplankton
2,000	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Freshwater invertebrates
Compound: Copper			Recommended BCF Value: 3,718
The BCF value was calculated using the geometric mean of 9 field values as follows:			
546	Namminga and Wilhm (1977)	Field samples.	*Chironomidae*
2,896 3,066 5,111 4,940 11,130 4,174 8,347 2,862	Saiki, Castleberry, May, Martin, and Bullard (1995)	Field samples.	*Chironomidae*; *Ephemeroptera*

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
373	Eisler (1977)	14-day exposure duration	*Mya arenara*
17,720 22,571	Graney, Cherry, and Cairns (1983)	28-day exposure duration	*Corbicula fluminea*
54 53 87 48 70 57 35 44	Jones, Jones and Radlett (1976)	25-day exposure duration	*Nereis diversicolor*
800	Majori and Petronio (1973)	8-day exposure duration	*Mytilus galloprovincialis*
104 2,792	McLusky and Phillips (1975)	21-day exposure duration	*Phylloduce maculata*
37 40 43 42	Nehring (1976)	14-day exposure duration; the value reported was converted to wet weight using a conversion factor of 5.99[(a)].	*Pteronarcys californica*
2,462	Pesch and Morgan (1978)	28-day exposure duration	*Nereis arenaceodentata*
35 185.5 69 26.5	Phillips (1976)	35-day exposure duration; the reported value was calculated by dividing the wet tissue concentration by the medium concentration [(µg/g)/(µg/L)], a conversion factor of 1 x 10^3 was applied to the value.	*Mytilus edulis*
5,160 11,800 6,800 19,000 11,560 27,800 12,540 22,500	Shuster and Pringle (1968)	35, 70, 105, and 140-day exposure duration	*Crassostrea virginica*
160	Pringle, Hissong, Katz, and Mulawka (1968)	70-day exposure duration	*Mya arenaria*
Compound: Cyanide (total)			Recommended BCF Value: 4,066
Laboratory data were not available for this constituent. The recommended BCF is the arithmetic mean of the recommended values for 14 inorganics with laboratory data available (antimony, arsenic, barium, beryllium, cadmium, chromium, copper, lead, mercury, nickel, selenium, silver, thallium, and zinc).			
Compound: Lead			Recommended BCF Value: 5,059
The BCF value was calculated using the geometric mean of 6 field values as follows:			

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

(Page 15 of 18)

Reported Values[a]	Reference	Experimental Parameters	Species
8,076 7,237 3,636 3,575 5,671 3,890	Nehring, Nisson, and Minasian (1979)	Field samples.	*Tipulidae*; *Para quetina* sp.; *Heptageniidae; Nemoura* sp.; *Macronenum* sp.; *Anisoptera*
2500	Borgmann, Kramar, and Loveridge (1978)	120-day exposure duration	*Lymnaea palustris*
357	Eisler (1977)	14-day exposure duration	*Mya arenara*
111 50 63 71 63	Nehring (1976)	14-day exposure duration; the reported value was converted from dry weight to wet weight using a conversion factor of 5.99[(a)].	*Petronarcys californica*
1520 502.5 765 555	Phillips (1976)	35-day exposure duration; the reported value was calculated by dividing the wet tissue concentration by the medium concentration [(µg/g)/(µg/L)], and an unit conversion factor of 1 x 10^3 was applied to the value.	*Mytilus edulis*
578 1,097	Zaroogian, Morrison, Heltshe (1979)	20-day exposure duration; The reported value was calculated by dividing the dry tissue concentration by the medium concentration [(µg/g)/(µg/kg)], and an unit conversion factor of 1 x 10^3 was applied to the value. A conversion factor or 5.99[(a)] was used to convert dry weight to wet weight.	*Crassostrea virginica*
Compound: Mercuric chloride			Recommended BCF Value: 20,184
The BCF value was based on 6 laboratory values as follows:			
100,000	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Marine and freshwater invertebrates
12,000	Kopfter (1974)	74-day exposure duration; the reported value was calculated by dividing the dry tissue concentration by the medium concentration [(ppm)/(ppb)], and an unit conversion factor of 1 x 10^3 was applied to the value.	*Crassostrea virginica*
13,633 14,600 14,217 19,916	Thurberg, Calabrese, Gould, Greig, Dawson, and Tucker (1977)	30 to 60-day exposure duration; The reported value was calculated by dividing the dry tissue concentration by the medium concentration [(ppm)/(ppb)], and an unit conversion factor of 1 x 10^3 was applied to the value.	*Homarus americanus*

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
Compound: Methyl mercury			Recommended BCF Value: 55,000
The BCF value was based on 1 laboratory value as follows:			
55,000	Kopfter (1974)	74-day exposure duration; The reported value was calculated by dividing the dry tissue concentration by the medium concentration [(ppm)/(ppb)] and a conversion factor of 1 x 10^3 was applied to the value.	*Crassostrea virginica*
Compound: Nickel			Recommended BCF Value: 28
The BCF value was calculated using the geometric mean of 4 laboratory values as follows:			
100 250	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Freshwater and marine invertebrates
2 12	Watras, MacFarlane, and Morel (1985)	Reported values adopted from a high and low range.	*Daphnia magna*
Compound: Selenium			Recommended BCF Value: 1,262
The BCF value was calculated using the geometric mean of 5 laboratory values as follows:			
229,000	Besser, Canfield, and LaPoint (1993)	96-hour exposure duration	*Daphnia magna*
90 930	Hermanutz, Allen, Roush, and Hedtke (1992)	365-day exposure duration	*Lepomis macrochirus*
167 1,000	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Freshwater and marine invertebrates
Compound: Silver			Recommended BCF Value: 298
The BCF value was calculated using the geometric mean of 12 laboratory values as follows:			
1,391 5,100 2,203 1,056 6,500 1,435	Calabrese, MacInnes, Nelson, Greig, and Yevich (1984)	540 to 630 day exposure duration; he reported value was calculated by dividing the wet tissue concentration by the medium concentration [(mg/kg)/(µg/L)], and an unit conversion factor of 1 x 10^3 was applied to the value.	*Mytilus edulis*

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
1,711	Metayer, Amiard-Triquet and Baud (1990)	14-day exposure duration	*Crassostrea gigas*
30 22 18 13 12	Nehring (1976)	14-day exposure duration; the reported value in Nehring (1976) was converted from dry weight to wet weight using a conversion factor of 5.99[(a)].	*Pteronarcys californica*
Compound: Thallium			Recommended BCF Value: 15,000
The BCF value was calculated using the geometric mean of 2 laboratory values as follows:			
15,000 15,000	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Freshwater and marine invertebrates
Compound: Zinc			Recommended BCF Value: 4,578
The BCF value was calculated using the geometric mean of 9 field values as follows:			
30,036	Namminga and Wilhm (1977)	Field samples.	*Chironomidae* sp.
2,613 2,199 1,282 3,210 4,718 6,625 3,876 10,274	Saiki, Castleberry, May, Martin, and Bullard (1995)	Field samples; the reported value was converted from dry weight to wet weight using a conversion factor of 5.99[(a)].	*Chironomidae* sp.; *Ephemeroptera* sp.
50 3,000	Deutch, Borg, Kloster, Meyer, and Moller (1980)	9-day exposure duration	Marine invertebrates
143	Eisler (1977)	14-day exposure duration	*Mya arenaria*
358 511 631	Graney, Cherry, and Cairns (1983)	28-day exposure duration	*Corbicula fluminea*
499 326 159 92 43 95 53 25 15 7	Nehring (1976)	14-day exposure duration; the reported value was converted from dry weight to wet weight using a conversion factor of 5.99[(a)].	*Ephemerella grandis*; *Pteronarcys californica*

TABLE C-3

WATER-TO-AQUATIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
519 2,615 315 184	Phillips (1976)	35-day exposure duration	Mytilus edulis
85	Pringle, Hissong, Katz, and Mulawka (1968)	50-day exposure duration	*Mya arenaria*

Notes:

(a) The reported values are presented as the amount of COPC in invertebrate tissue divided by the amount of COPC in the water. If the values reported in the studies were presented as dry tissue weight over amount of COPC in water, they were converted to wet weight by dividing the concentration in dry invertebrate tissue weight by 5.99. This conversion factor assumes an invertebrate's total weight is 83.3 percent moisture, which is based on the moisture content of the earthworm (Pietz et al. 1984).

The conversion factor was calculated as follows:

$$Conversion\ factor = \frac{1.0\ gram\ (g)\ invertebrate\ total\ weight}{1.0\ gram\ (g)\ invertebrate\ total\ weight\ -\ 0.833\ g\ invertebrate\ wet\ weight}$$

(b) Reported field values for organic COPCs are assumed to be total COPC concentration in water and, therefore, were converted to dissolved COPC concentration in water using the following equation from U.S.EPA (1995b):

$BCF\ (dissolved) = (BCF\ (total) / f_{fd}) - 1$

where: BCF (dissolved) = BCF based on dissolved concentration of COPC in water
BCF (total) = BCF based on the field derived data for total concentration of COPC in water
f_{fd} = Fraction of COPC that is freely dissolved in the water

where: $f_{fd} = 1 / [1 + ((DOC \times K_{ow}) / 10) + (POC \times K_{ow})]$
DOC = Dissolved organic carbon, kilograms of organic carbon / liter of water (2.0×10^{-06} Kg/L)
K_{ow} = Octanol-water partition coefficient of the COPC, as reported in U.S. EPA (1994b)
POC = Particulate organic carbon, kilograms of organic carbon / liter of water (7.5×10^{-09} Kg/L)

TABLE C-4

WATER-TO-ALGAE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
Dioxins and Furans			
Compound: 2,3,7,8-Tetrachlorodibenzo(p)dioxin (2,3,7,8-TCDD)			Recommended BCF value: 3,302
The recommended BCF value was calculated using the geometric mean of 3 laboratory values as follows:			
4,000 9,000	Yockim, Isensee, and Jones (1978)	Values adopted from a high to low range; reported values were for 2,3,7,8-tetrachlorodibenzo(p)dioxin (2,3,7,8-TCDD).	*Leona minor*
1,000	Yockim, Isensee, and Jones (1978)	32-day exposure duration; reported values were for 2,3,7,8-TCDD.	*Oedogonium cardiacum*
Compound: 1,2,3,7,8-Pentachlorodibenzo(p)dioxin (1,2,3,7,8-PeCDD)			Recommended BCF value: 3,038
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 3,302 x 0.92 = 3,038			
Compound: 1,2,3,4,7,8-Hexachlorodibenzo(p)dioxin (1,2,3,4,7,8-HxCDD)			Recommended BCF value: 1,024
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 3,302 x0.31 = 1,024			
Compound: 1,2,3,6,7,8-Hexachlorodibenzo(p)dioxin (1,2,3,6,7,8-HxCDD)			Recommended BCF value: 396.2
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 3,302 x0.12 = 396.2			
Compound: 1,2,3,7,8,9-Hexachlorodibenzo(p)dioxin (1,2,3,7,8,9-HxCDD)			Recommended BCF value: 462.3
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 3,302 x0.14 = 462.3			
Compound: 1,2,3,4,6,7,8-Heptachlorodibenzo(p)dioxin (1,2,3,4,6,7,8-HpCDD)			Recommended BCF value: 168.4
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 3,302 x0.051 = 168.4			
Compound: Octachlorodibenzo(p)dioxin (OCDD)			Recommended BCF value: 39.6
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 3,302 x0.012 = 39.6			
Compound: 2,3,7,8-Tetrachlorodibenzofuran (2,3,7,8-TCDF)			Recommended BCF value: 2,642
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 3,302 x0.80 = 2,642			
Compound: 1,2,3,7,8-Pentachlorodibenzofuran 1,(2,3,7,8-PeCDF)			Recommended BCF value: 726.4
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 3,302 x0.22 =726.4			

TABLE C-4

WATER-TO-ALGAE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
Compound: 2,3,4,7,8-Pentachlorodibenzofuran (2,3,4,7,8-PeCDF)			Recommended BCF value: 5,283
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 3,302 x1.6 = 5,283			
Compound: 1,2,3,4,7,8-Hexachlorodibenzofuran (1,2,3,4,7,8-HxCDF)			Recommended BCF value: 251.0
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 3,302 x 0.076 = 251.0			
Compound: 1,2,3,6,7,8-Hexachlorodibenzofuran (1,2,3,6,7,8-HxCDF)			Recommended BCF value: 627.4
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 3,302 x0.19 = 627.4			
Compound: 2,3,4,6,7,8-Hexachlorodibenzofuran (2,3,4,6,7,8-HxCDF)			Recommended BCF value: 2,212
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 3,302 x0.67 = 2,212			
Compound: 1,2,3,7,8,9-Hexachlorodibenzofuran (1,2,3,7,8,9-HxCDF)			Recommended BCF value: 2,080
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 3,302 x 0.63 = 2,080			
Compound: 1,2,3,4,6,7,8-Heptachlorodibenzofuran (1,2,3,4,6,7,8-HpCDF)			Recommended BCF value: 36.3
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 3,302 x0.011 = 36.3			
Compound: 1,2,3,4,7,8,9-Heptachlorodibenzofuran (1,2,3,4,7,8,9-HpCDF)			Recommended BCF value: 1,288
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 3,302 x0.39 = 1,288			
Compound: Octachlorodibenzofuran (OCDF)			Recommended BCF value: 52.8
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF = 3,302 x 0.016 = 52.8			
Polynuclear Aromatic Hydrocarbons (PAHs)			
Compound: Benzo(a)pyrene			Recommended BCF value: 5,258
The recommended BCF value was based on a single measured value for benzo(a)pyrene. This value was also used as a surrogate for all high molecular weight PAHs for which laboratory data were not available.			
5,258	Lu, Metcalf, Plummer, and Mandel (1977)	3-day exposure duration	*Oedogonium cardiacum*
Compound: Benzo(a)anthracene			Recommended BCF value: 5,258

TABLE C-4

WATER-TO-ALGAE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
Laboratory data were not available for this compound. The BCF for benzo(a)pyrene was used as a surrogate.			
Compound: Benzo(b)fluoranthene			Recommended BCF value: 5,258
Laboratory data were not available for this compound. The BCF for benzo(a)pyrene was used as a surrogate.			
Compound: Benzo(k)fluoranthene			Recommended BCF value: 5,258
Laboratory data were not available for this compound. The BCF for benzo(a)pyrene was used as a surrogate.			
Compound: Chrysene			Recommended BCF value: 5,258
Laboratory data were not available for this compound. The BCF for benzo(a)pyrene was used as a surrogate.			
Compound: Dibenz(a,h)anthracene			Recommended BCF value: 5,258
Laboratory data were not available for this compound. The BCF for benzo(a)pyrene was used as a surrogate.			
Compound: Indeno(1,2,3-cd)pyrene			Recommended BCF value: 5,258
Laboratory data were not available for this compound. The BCF for benzo(a)pyrene was used as a surrogate.			
Polychlorinated Biphenyls (PCBs)			
Compound: Aroclor 1016			Recommended BCF value: 476,829
The reported value was calculated by dividing the wet tissue concentration by the medium concentration (ppm/pptr). A conversion factor of 1×10^6 was applied to the value. The BCF value is based on Aroclor 1254 since there was no available data for total PCB.			
476,829	Scura and Theilacker (1977)	45-day exposure to Aroclor 1254	*Dunaliella* sp.
Compound: Aroclor 1254			Recommended BCF value: 476,829
The reported value was calculated by dividing the wet tissue concentration by the medium concentration (ppm/pptr). A conversion factor of 1×10^6 was applied to the value. The BCF value is based on Aroclor 1254 since there was no available data for total PCB.			
476,829	Scura and Theilacker (1977)	45-day exposure to Aroclor 1254	*Dunaliella* sp.

TABLE C-4

WATER-TO-ALGAE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
Nitroaromatics			
Compound: 1,3-Dinitrobenzene			Recommended BCF value: 2,507
Laboratory data were not available for this compound. The BCF for 2,4-dinitrotoluene was used as a surrogate.			
Compound: 2,4-Dinitrotoluene			Recommended BCF value: 2,507
The recommended BCF value was based on one study as follows:			
2,507	Liu, Bailey, and Pearson (1983)	4-day exposure duration	*Selanastrum capricornatum*
Compound: 2,6-Dinitrobenzene			Recommended BCF value: 2,507
Laboratory data were not available for this compound. The BCF for 2,4-dinitrotoluene was used as a surrogate.			
Compound: Nitrobenzene			Recommended BCF value: 24
The recommended BCF value was based on one study as follows:			
24	Geyer, Viswanathan, Freitag, and Korte (1981)	1-day exposure duration	*Chlorella fusca*
Compound: Pentachloronitrobenzene			Recommended BCF value: 4,740
The recommended BCF value calculated using the geometric mean of 4 laboratory values as follows:			
3,100	Geyer, Viswanathan, Freitag, and Korte (1981)	1-day exposure duration	*Chlorella fusca*
4,795 7,534	Korte, Freitag, Geyer, Klein, Kraus, and Lahaniatis (1978)	1-day exposure duration; The values reported in Korte, Freitag, Geyer, Klein, Kraus, and Lahaniatis (1978) were converted to wet weight using a conversion factor of 2.92 [a].	*Chlorella fusca*
4,508	Wang, Harada, Watanabe, Koshikawa, and Geyer (1996)	Not reported	*Chlorella fusca*
Phthalate Esters			
Compound: Bis(2-ethylhexyl)phthalate			Recommended BCF value: 9,931

TABLE C-4

WATER-TO-ALGAE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
The recommended BCF value was calculated using the geometric mean of 2 laboratory values as follows:			
5,400	Geyer, Viswanathan, Freitag, and Korte (1981)	1-day exposure duration	*Chlorella fusca*
18,263	Sodergren (1982)	27-day exposure duration	*Chara chara*
Compound: Di(n)octyl phthalate			Recommended BCF value: 28,500
The recommended BCF value was based on one study as follows:			
28,500	Sanborn, Metcalf, Yu, and Lu (1975)	33-day exposure duration	*Oedogonium cardiacum*
Volatile Organic Compounds			
Compound: Acetone			Recommended BCF value: 0.05
Laboratory data were not available for this compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = -0.222 (Karickoff and Long 1995)			
Compound: Acrylonitrile			Recommended BCF value: 0.11
Laboratory data are not available for this compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 0.250 (Karickoff and Long 1995)			
Compound: Chloroform			Recommended BCF value: 2.82
Laboratory data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 1.949 (U.S. EPA 1994b)			
Compound: Crotonaldehyde			Recommended BCF value: 0.20
Laboratory data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 0.55 (based on equation developed by Hansch and Leo 1979, calculated in NRC (1981))			
Compound: 1,4-Dioxane			Recommended BCF value: 0.04
Laboratory data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = -0.268 (U.S. EPA 1995a)			
Compound: Formaldehyde			Recommended BCF value: 0.14

TABLE C-4

WATER-TO-ALGAE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
Laboratory data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 0.342 (U.S. EPA 1995a)			
Compound: Vinyl chloride			Recommended BCF value: 0.62
Laboratory data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 1.146 (U.S. EPA 1994b)			
Other Chlorinated Organics			
Compound: Carbon tetrachloride			Recommended BCF value: 300
The recommended BCF value was based on laboratory data as follows:			
300	Geyer, Politzki and Freitag (1984)	1-day exposure duration	*Chlorella fusca*
Compound: Hexachlorobenzene			Recommended BCF value: 11,134
The recommended BCF value was calculated using the geometric mean of 4 laboratory values as follows:			
24,800	Geyer, Politzki, and Freitag (1984)	1-day exposure duration	*Chlorella fusca*
610	Isensee, Holden, Woolson and Jones (1976)	31-day exposure duration	*Oedogonium cardiacum*
41,096	Korte, Freitag, Geyer, Klein, Kraus, and Lahaniatis (1978)	1-day exposure duration; the values reported in Korte, Freitag, Geyer, Klein, Kraus, and Lahaniatis (1978) were converted to wet weight using an unit conversion factor of 2.92 [a] .	*Chlorella fusca*
24,717	Wang, Harada, Watanabe, Koshikawa, and Geyer (1996)	Not reported	*Chlorella fusca*
Compound: Hexachlorobutadiene			Recommended BCF value: 160
The recommended BCF value calculated using the geometric mean of 2 laboratory values as follows:			
160	Laseter, Bartell, Laska, Holmquist, Condie, Brown, and Evans (1976)	7-day exposure duration	*Oedogonium cardiacum*
160	U.S. EPA (1976)	Not reported	Algae
Compound: Hexachlorocyclopentadiene			Recommended BCF value: 610

TABLE C-4

WATER-TO-ALGAE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
The recommended BCF value was calculated using the geometric mean of 2 laboratory values as follows:			
1,090	Geyer, Viswanathan, Freitag, and Korte (1981)	Not reported	*Chlorella fusca*
341	Lu, Metcalf, Hirwe, and Williams (1975)	Not reported	*Oedogonium cardiacum*
Compound: Pentachlorobenzene			Recommended BCF value: 4,000
The recommended BCF value was based on one study as follows:			
4,000	Geyer, Politzki, and Freitag (1984)	1-day exposure duration	*Chlorella fusca*
Compound: Pentachlorophenol			Recommended BCF value: 1,711
The recommended BCF value calculated using the geometric mean of 4 laboratory values as follows:			
1,250	Geyer, Viswanathan, Freitag, and Korte (1981)	1-day exposure duration	*Chlorella fusca*
2,055 2,534 1,781	Korte, Freitag, Geyer, Klein, Kraus, and Lahaniatis (1978)	1-day exposure duration; the values reported in Korte, Freitag, Geyer, Klein, Kraus, and Lahaniatis (1978) were converted to wet weight using an unit conversion factor of 2.92 [a].	*Chlorella fusca*
1,266	Wang, Harada, Watanabe, Koshikawa, and Geyer (1996)	Not reported	*Chlorella fusca*
Pesticides			
Compound: 4,4'-DDE			Recommended BCF value: 11,251
The recommended BCF value was based on one study as follows:			
11,251	Metcalf, Sanborn, Lu, and Nye (1975)	33-day exposure duration	*Oedogonium cardiacum*
Compound: Heptachlor			Recommended BCF value: 21,000
The recommended BCF value was based on one study as follows:			
21,000	U.S. EPA (1979)	Not reported	Algae

TABLE C-4

WATER-TO-ALGAE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
Compound: Hexachlorophene			Recommended BCF value: 1,500
The recommended BCF value was based on one study as follows:			
1,500	Sanborn (1974)	Not reported	Algae
Inorganics			
Compound: Aluminum			Recommended BCF value: 833
The recommended BCF value was based on one study as follows:			
600	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Algae (marine plants)
Compound: Antimony			Recommended BCF value: 1,475
The recommended value was calculated using the geometric mean of 2 laboratory values as follows:			
1,500 1,450	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Not reported
Compound: Arsenic			Recommended BCF value: 293
The recommended value was calculated using the geometric mean of 3 laboratory values as follows:			
5	Anderson et al. (1979)	42-day exposure duration	*Lemna minor*
3,000 1,670	Thompson, Burton, Quinn, and Ng 1972	Not reported	Not reported
Compound: Barium			Recommended BCF value: 260
The recommended BCF value was based on one study as follows:			
260	Schroeder (1970)	Not reported	Brown algae
Compound: Beryllium			Recommended BCF value: 141
The recommended value was calculated using the geometric mean of 2 laboratory values as follows:			
20 1,000	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Not reported

TABLE C-4

WATER-TO-ALGAE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
Compound: Cadmium			Recommended BCF value: 782
The recommended BCF value was calculated using the geometric mean of 6 laboratory values as follows:			
300 1,000 370 1,000	Fisher, Bohe, and Teyessie (1984)	Not reported	*Thalassiosira pseudonana* *Dunaliella tertiolecta* *Emiliania huxleyi* *Oscillatoria woronichinii*
2,065	Hutchinson and Czyrska (1972)	21-day exposure duration; The values reported in Hutchinson and Czyrska (1972) were converted to wet weight using a conversion factor of 2.92 [a].	*Lemna valdiviana*
1,000	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Not reported
Compound: Chromium (total)			Recommended BCF value: 4,406
The recommended BCF value was calculated using the geometric mean of 8 laboratory values as follows:			
343	Jouany, Vasseur, and Ferard (1982)	28-day exposure duration; the values reported in Jouany, Vasseur, and Ferard (1982) were converted to wet weight using an unit conversion factor of 2.92 [a].	*Chlorella vulgaris*
1,600	NAS (1974)	Not reported	Benthic algae
26,316 8,485 29,000 5,000	Patrick, Bott, and Larson (1975)	4 experiments consisting of 1-month exposure durations	Mixed algae
4,000 2,000	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Not reported
Compound: Copper			Recommended BCF value: 541
The recommended BCF value was calculated using the geometric mean of 5 laboratory values as follows:			
17	Bastien and Cote (1989)	50-day exposure duration	*Scenedesmus quadricauda*
827 1,644	Stokes, Hutchinson, and Krauter (1973)	2-day exposure duration	*Scenedesmus* sp.

TABLE C-4

WATER-TO-ALGAE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
2,000 1,000	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Freshwater and marine plants
Compound: Cyanide (total)			Recommended BCF value: 22
The recommended BCF value was based on one study as follows:			
22	Low and Lee (1981)	72-hour exposure duration	*Eichhornia crassipes*
Compound: Lead			Recommended BCF value: 1,706
The recommended BCF value was calculated using the geometric mean of 3 laboratory values as follows:			
100 5,000	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Not reported
9,931	Vighi (1981)	28-day exposure duration; the values reported in Vighi (1981) were converted to wet weight using an unit conversion factor of 2.92 [a].	*Selenastrum capricornutum*
Compound: Mercury chloride			Recommended BCF value: 24,762
The recommended BCF value was based on one study as follows:			
24,762	Watras and Bloom (1992)	Field samples	Phytoplankton
Compound: Methyl mercury			Recommended BCF value: 80,000
The recommended BCF value was based on one study as follows:			
80,000	Watras and Bloom (1992)	Field samples	Phytoplankton
Compound: Nickel			Recommended BCF value: 61
The recommended BCF value was calculated using the geometric mean of 4 laboratory values as follows:			
32 34	Hutchinson and Stokes (1975)	6-day exposure duration	*Scenedesmus* sp.
50 250	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Not reported

TABLE C-4

WATER-TO-ALGAE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
Compound: Selenium			Recommended BCF value: 1,845
The recommended BCF value was calculated using the geometric mean of 3 laboratory values as follows:			
15,700	Besser, Canfield, and LaPoint (1993)	24-hour exposure duration	*Chlamydomonas reinhardtii*
400	Dobbs, Cherry, and Cairns (1996)	25-day exposure duration	*Chlorella vulgaris*
1,000	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Not reported
Compound: Silver			Recommended BCF value: 10,696
The recommended BCF value was calculated using the geometric mean of 5 laboratory values as follows:			
34,000 13,000 24,000 66,000	Fisher, Bohe, and Teyssie (1984)	Not reported	*Thalassiosira pseudonana* *Dunaliella tertiolecta* *Emiliania huxleyi* *Oscillatoria woronichinii*
200	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Not reported
Compound: Thallium			Recommended BCF value: 15,000
The recommendedBCF was based on one study as follows:			
15,000	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Not reported
Compound: Zinc			Recommended BCF value: 2,175
The recommended BCF value was calculated using the geometric mean of 17 laboratory values as follows:			
285 4,395	Andryushhenko and Polikarpou (1973)	5-day exposure duration	*Ulva rigida*
4,680	Baudin (1974)	34-day exposure duration	*Cladophoea*
70 600 1,200 1,400 170,000	Deutch, Borg, Kloster, Meyer, and Moller (1980)	9-day exposure duration	*Codium fragile* *Enteromorpha* sp. *Ulva lactuca* *Fucus serratus* Marine plankton

TABLE C-4

WATER-TO-ALGAE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values[a]	Reference	Experimental Parameters	Species
12,000 10,000 4,600 5,200	Fisher, Bohe, and Teyssie (1984)	Not reported	*Thalassiosira pseudonana* *Dunaliella tertiolecta* *Emiliania huxleyi* *Oscillatoria woronichinii*
524 1,015	Munda (1979)	12-day exposure; The values reported in Munda (1979) were converted to wet weight using a conversion factor of 2.92 [a].	*Enteromorpha prolifera* *Fucus vivsoides*
255	U.S. EPA (1987a)	6-day exposure duration	*Ulva lactuca*
20,000 1,000	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Not reported

Notes:

(a) The reported values are presented as the amount of COPC in algae divided by the amount of COPC in water. If the values reported in the studies were presented as dry tissue weight over the amount of COPC in water, they were converted to wet weight over dry weight by dividing the concentration in dry algae tissue weight by 2.92. This conversion factor assumes an algae total weight is 65.7 percent moisture (Isensee, Kearney, Woolson, Jones and Williams 1973). The conversion factor was calculated as follows:

$$Conversion\ factor = \frac{1.0\ g\ algae\ total\ weight}{1.0\ g\ algae\ total\ weight - 0.675\ g\ algae\ wet\ weight}$$

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values	Reference	Experimental Parameters	Species
Dioxins and Furans			
Compound: 2,3,7,8-Tetrachlorinated dibenzo(p)dioxin (2,3,7,8-TCDD)			Recommended BCF value: 4,235
The recommended value was calculated using the geometric mean of 12 laboratory values for several PCDD compounds as follows:			
5,800	Adams, DeGraeve, Sabourin, Cooney, and Mosher (1986)	28-day exposure duration, 20-day elimination; reported data were for 2,3,7,8-tetrachlorodibenzo(p)dioxin (2,3,7,8-TCDD)	*Pimephales promelas*
9,270	Branson, Takahashi, Parker, and Blau (1985)	6-hour exposure duration, 139-day depuration	*Oncorhynchus mykiss*
39,000	Mehrle, Buckler, Little, Smith, Petty, Peterman, Stalling, DeGraeve, Coyle, and Adams (1988)	28-day exposure duration	*Oncorhynchus mykiss*
810 2,840 513 5,834	Muir, Marshall, and Webster (1985)	4 to 5-day exposure duration, 24 to 28-day depuration; values are based on a high to low range of reported values.	*Oncorhynchus mykiss* *Pimephales promelas*
2,769 2,269	Yockim, Isensee, and Jones (1978)	15-day exposure duration	*Gambusia affinis* *Ictalurus* sp.
5,000 9,300 7,900	U.S. EPA (1985)	Not reported	*Pimephales promelas*
Compound: 1,2,3,7,8-Pentachlorodibenzo(p)dioxin (1,2,3,7,8-PeCDD)			Recommended BCF value: 3,896
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =4,235 x 0.92 =3,896			
Compound: 1,2,3,4,7,8-Hexachlorodibenzo(p)dioxin (1,2,3,4,7,8-HxCDD)			Recommended BCF value: 1,313
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =4,235 x 0.31 =1313			
Compound: 1,2,3,6,7,8-Hexachlorodibenzo(p)dioxin (1,2,3,6,7,8-HxCDD)			Recommended BCF value: 508.2
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =4,235 x 0.12 =508.2			

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values	Reference	Experimental Parameters	Species
Compound: 1,2,3,7,8,9-Hexachlorodibenzo(p)dioxin (1,2,3,7,8,9-HxCDD)		Recommended BCF value:	592.9
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =4,235 x 0.14 =592.9			
Compound: 1,2,3,4,6,7,8-Heptachlorodibenzo(p)dioxin (1,2,3,4,6,7,8-HpCDD)		Recommended BCF value:	215.9
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =4,235 x 0.051 =215.9			
Compound: Octachlorodibenzo(p)dioxin (OCDD)		Recommended BCF value:	50.8
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =4,235 x 0.012 =50.8			
Compound: 2,3,7,8-Tetrachlorinated dibenzofuran (2,3,7,8-TCDF)Compound:		Recommended BCF value:	3,388
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =4,235 x 0.80 =3,388			
Compound: 1,2,3,7,8-Pentachlorodibenzo(p)furan (1,2,3,7,8-PeCDF)		Recommended BCF value:	931.7
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =4,235 x 0.22 =931.7			
Compound: 2,3,4,7,8-Pentachlorodibenzo(p)furan (2,3,4,7,8-PeCDF)		Recommended BCF value:	6,776
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =4,235 x1.6 =6,776			
Compound: 1,2,3,4,7,8-Hexachlorodibenzo(p)furan (1,2,3,4,7,8-HxCDF)		Recommended BCF value:	3,21.9
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =4,235 x 0.076 =3,21.9			
Compound: 1,2,3,6,7,8-Hexachlorodibenzo(p)furan (1,2,3,6,7,8-HxCDF)		Recommended BCF value:	804.7
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =4,235 x 0.19 =804.7			
Compound: 2,3,4,6,7,8-Hexachlorodibenzo(p)furan (2,3,4,6,7,8-HxCDF)		Recommended BCF value:	2,837
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =4,235 x 0.67 = 2,837			
Compound: 1,2,3,7,8,9-Hexachlorodibenzo(p)furan (1,2,3,7,8,9-HxCDF)		Recommended BCF value:	2,668
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =4,235 x 0.63 =2,668			

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values	Reference	Experimental Parameters	Species
Compound: 1,2,3,4,6,7,8,-Heptachlorodibenzo(p)furan (1,2,3,4,6,7,8-HpCDF)			Recommended BCF value: 46.6
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =4,235 x 0.011 =46.6			
Compound: 1,2,3,4,7,8,9-Heptachlorodibenzo(p)furan (1,2,3,4,7,8,9-HpCDF)			Recommended BCF value: 1,651
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =4,235 x 0.39 =1,651			
Compound: Octachlorodibenzo(p)furan (OCDF)			Recommended BCF value: 67.8
The BCF was calculated using the TCDD BCF and a bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =4,235 x 0.016 =67.8			
Polynuclear Aromatic Hydrocarbons (PAHs)			
Compound: Benzo(a)pyrene			Recommended BCF value: 500
The recommended value is that presented in Stephan (1993), which was the geometric mean of 16 laboratory values. This BCF for benzo(a)pyrene is also recommended for high molecular weight PAH for which empirical data are not available.			
500	Stephan (1993)	Not reported	Not reported
Compound: Benzo(a)anthracene			Recommended BCF value: 500
Empirical data were not available for this compound. The BCF for benzo(a)pyrene was used as a surrogate.			
Compound: Benzo(b)fluoranthene			Recommended BCF value: 500
Empirical data were not available for this compound. The BCF for benzo(a)pyrene was used as a surrogate.			
Compound: Benzo(k)fluoranthene			Recommended BCF value: 500
Empirical data were not available for this compound. The BCF for benzo(a)pyrene was used as a surrogate.			
Compound: Chrysene			Recommended BCF value: 500
Empirical data were not available for this compound. The BCF for benzo(a)pyrene was used as a surrogate.			
Compound: Dibenz(a,h)anthracene			Recommended BCF value: 500
Empirical data were not available for this compound. The BCF for benzo(a)pyrene was used as a surrogate.			

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values	Reference	Experimental Parameters	Species
Compound: Indeno(1,2,3-cd)pyrene			Recommended BCF value: 500
Empirical data were not available for this compound. The BCF for benzo(a)pyrene was used as a surrogate.			
Polychlorinated Biphenyls (PCBs)			
Compound: Aroclor 1016			Recommended BCF value: 22,649
The recommended BCF value was calculated using the geometric mean of 4 field values as follows[b, c, d]:			
25,000	Hansen et al. (1975) as cited in U.S. EPA (1980b)	28 days exposure 1.1 percent lipid Adult	*Cyprinodon variegatus*
43,000	Hansen et al. (1975) as cited in U.S. EPA (1980b)	28 days exposure Whole body Juvenile	*Cyprinodon variegatus*
14,400	Hansen et al. (1975) as cited in U.S. EPA (1980b)	28 days exposure Whole body Fry	*Cyprinodon variegatus*
17,000	Hansen et al. (1974) as cited in U.S. EPA (1980b)	21 to 28 days exposure Whole body	*Lagodon rhomboides*
Compound: Aroclor 1254			Recommended BCF value: 230,394
The recommended BCF value was calculated using the geometric mean of 7 field values as follows[b, c, d]:			
238,000 females 235,000 males	Nebeker, Puglisi, and DeFoe (1974)	Fish exposed for eight months. Residues measured in males and females.	*Pimephales promeles*
35,481 354,813 281,838	Rice and White (1987)	Field study	*Pimephales promeles*
46,000	Bills and Marking (1987)	30-day exposure duration Whole body	*Oncorhynchus mykiss*

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values	Reference	Experimental Parameters	Species
13,000,000 in lipid 1,030,000 dry tissue	Scura and Theilacker (1977)	45 days exposure	*Engraulis mordex*
370,000 1,200,000	Veith et al. (1977)	Field samples	Sculpins (bottom fish) Pelagic fish
47,000	Mauck et al. (1978) as cited in U.S. EPA (1980b)	118 days exposure Whole body	*Salvellnus fontinalis*
42,000	Snarski and Puglisi (1976) as cited in U.S. EPA (1980b)	500 days exposure Body lipid 2.9 percent Whole body	*Salvellnus fontinalis*
37,000	Hansen et al. (1971) as cited in EPA (1980b)	28 days exposure 1.1 percent lipid Whole body	*Leiostomus xanthurus*
30,000	Hansen et al. (1973) as cited in EPA (1980b)	28 days exposure 3.6 percent lipid Whole body	*Cyprinodon variegatus*
>670,00	Duke et al. (1970) and Nimmo et al. (1977) as cited in EPA (1980b)	Field data Whole body	*Cynoscion nebulosus*
>133,000	Nimmo et al. (1977) as cited in EPA (1980b)	Field data	Fishes
38,000	Halter (1974) as cited in EPA (1980b)	24 days exposure	*Salmo gairdneri*
61,200	Mayer et al. (1977) as cited in EPA (1980b)	77 days exposure Whole body	*Ictalurus punctatus*
Nitroaromatics			
Compound: 1,3-Dinitrobenzene			Recommended BCF value: 74
The BCF for 1,3 -dinitrobenzene was based on one laboratory value as follows:			
74	Deener, Sinnige, Seinen, and Hemens (1987)	3-day exposure duration	*Poecilia reticulata*
Compound: 2,4-Dinitrotoluene			Recommended BCF value: 21.04

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values	Reference	Experimental Parameters	Species
Empirical data for this compound were not available. The BCF for nitrobenzene was used as a surrogate.			
Compound: 2,6-Dinitrotoluene			Recommended BCF value: 21.04
Empirical data for this compound were not available. The BCF for nitrobenzene used as a surrogate.			
Compound: Nitrobenzene			Recommended BCF value: 21.04
The recommended BCF value was calculated using the geometric mean of 2 laboratory values as follows:			
29.5	Deneer, Sinnige, Seinen, and Hermens (1987)	3-day exposure duration	*Poecilia reticulata*
15	Veith, DeFoe, and Bergstedt (1979)	28-day exposure duration	*Pimephales promelas*
Compound: Pentachloronitrobenzene			Recommended BCF value: 214
The recommended BCF value was calculated using the geometric mean of 7 laboratory values as follows:			
238	Kanazawa (1981)	Continuous flow test	*Pseudorasbora parva*
250 320 380	Korte, Freitag, Geyer, Klein, Kraus, and Lahaniatis (1978)	24-hr exposure duration	*Leucisens idus melanotus*
114 147 169	Niimi, Lee, and Kissoon (1989)	20, 28, and 36-day exposure duration	*Oncorhynchus mykiss*
Phthalate Esters			
Compound: Bis(2-ethylhexyl)phthalate			Recommended BCF value: 70
The recommended BCF value was calculated using the geometric mean of 14 laboratory values as follows:			
91 569	Mayer (1976)	56-day exposure duration; based on a high to low range of reported values.	*Pimephales promelas*
155 42	Mehrle and Mayer (1976)	36 to 56-day exposure	*Pimephales promelas* *Oncorhynchus mykiss*

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values	Reference	Experimental Parameters	Species
178 10,563 306	Sodergren (1982)	27-day exposure duration	*Phoxinus phoxinus* *Lampetra planeri* *Pungitis pungitis*
51.5 8.9 1.6	Tarr, Barron, and Hayton (1990)	Not reported	*Salmo gairdneri*
4	U.S. EPA (1992a)	Not reported	Fish
851	Veith, DeFoe, and Bergstedt (1979)	Not reported	*Pimephales promelas*
10.7 13.5	Wofford, Wilsey, Neff, Giam, and Neff (1981)	24-hour exposure duration	*Cypinodon variegatus*
Compound: Di(n)octyl phthalate			Recommended BCF value: 9,400
The recommended BCF value was based on data from one study as follows:			
9,400	Sanborn, Metcalf, Yu, and Lu (1975)	Not reported	*Gambusia affinis*
Volatile Organic Compounds			
Compound: Acetone			Recommended BCF value: 0.10
Empirical data were not available for this compound. The BCF was calculated using the following regression equation: log BCF = 0.91 x log K_{ow} - 1.975 x log(6.8E-07 x K_{ow} + 1.0) - 0.786 (Bintein et al. 1993), where log K_{ow} = -0.222 (Karickoff and Long 1995)			
Compound: Acrylonitrile			Recommended BCF value: 48
The recommended BCF value was based on data from one study as follows:			
48	Barrows, Petrocelli, Macek, and Carroll (1978)	28-day exposure duration	*Lepomis macrochirus*
Compound: Chloroform			Recommended BCF value: 3.59
The recommended BCF value was calculated using the geometric mean of 3 laboratory values follows:			
5.6 3.44 2.4	Anderson and Lusty (1980)	24-hr exposure, 24-hr depuration	*Oncorhynchus mykiss* *Leponis macrochinus* *Micropterus salmoides*

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values	Reference	Experimental Parameters	Species
Compound: Crotonaldehyde			Recommended BCF value: 0.52
Empirical data were not available for this compound. The BCF was calculated using the following regression equation: log BCF = 0.91 x log K_{ow} - 1.975 x log(6.8E-07 x K_{ow} + 1.0) - 0.786 (Bintein et al. 1993), where log K_{ow} = 0.55 (based on equation in Hansch and Leo 1979, as calculated in NRC (1981)).			
Compound: Formaldehyde			Recommended BCF value: 0.34
Empirical data were not available for this compound. The BCF was calculated using the following regression equation: log BCF = 0.91 x log K_{ow} - 1.975 x log(6.8E-07 x K_{ow} + 1.0) - 0.786 (Bintein et al. 1993), where log K_{ow} = 0.342 (U.S. EPA 1995a)			
Compound: Vinyl chloride			Recommended BCF value: 1.81
Empirical data were not available for this compound. The BCF was calculated using the following regression equation: log BCF = 0.91 x log K_{ow} - 1.975 x log(6.8E-07 x K_{ow} + 1.0) - 0.786 (Bintein et al. 1993), where log K_{ow} =1.146 (U.S. EPA 1994b)			
Other Chlorinated Organics			
Compound: Carbon tetrachloride			Recommended BCF value: 30
The recommended BCF value was based on 1 laboratory values as follows:			
30	Barrows, Petrocelli, Macek, and Carroll (1978)	28-day exposure duration	*Lepomis macrochirus*
Compound: Hexachlorobenzene			Recommended BCF value: 253
The recommended BCF value on 1 field value as follows[b, c]			
253	Oliver and Niimi (1988)	Field samples.	Freshwater fish
22,000	Carlson and Kosian (1987)	32-day exposure duration	*Pimephales promelas*
1,260 2,040 6,160 15,850	Isensee, Holden, Woolson, and Jones (1976)	31-day exposure duration	*Gambusia affinis* *Ictalurus punctatus*
290,000	Koneman and van Leeuwen (1980)	Not reported	*Poecilia reticulata*
400 420	Korte, Freitag, Geyer, Klein, Kraus, and Lahaniatis (1978)	1-day exposure duration	*Zeucisens idus melanotus*

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values	Reference	Experimental Parameters	Species
32,000 39,000	Kosian, Lemke, Studders, and Veith (1981)	28-day exposure duration	*Pimephales promelas*
5,200 6,970	Lores, Patrick, and Summers (1993)	30-day exposure duration; based on a high to low range of reported values.	*Cyprinodon variegatus*
93 287	Metcalf, Kapoor, Lu, Schuth, and Sherman (1973)	3 to 32-day exposure duration	*Gambusia affinis*
12,240 12,600 15,250 13,330 21,140	Nebeker, Griffis, Wise, Hopkins, and Barbittas (1989)	28-day exposure duration	*Pimephales promelas*
253,333	Oliver and Niimi (1983)	119-day exposure duration	*Oncorhynchus mykiss*
27,000	Schrap and Opperhuizen (1990)	Not reported	*Poecilia reticulata*
18,500	Veith, DeFoe, and Bergstedt (1979)	32-day exposure duration	*Pimephales promelas*
7,800	U.S. EPA (1987)	Not reported	*Oncorhynchus mykiss*
8,690	U.S. EPA (1980h)	Not reported	*Pimephales promelas*
253	Oliver and Niimi (1988)	Field samples.	Freshwater fish
Compound: Hexachlorobutadiene			Recommended BCF value: 783
The recommended BCF value was calculated using the geometric mean of 3 laboratory values as follows:			
920 1,200	Leeuwangh, Bult, and Schneiders (1975)	49-day exposure duration; 15-day depuration. The values reported in Leeuwangh, Bult, and Schneiders (1975) were converted to wet weight using an unit conversion factor of 5.0 [a].	*Carassius auratus*
435	Laska, Bartell, Laseter (1976)	Not reported	*Gambusia affinis*
Compound: Hexachlorocyclopentadiene			Recommended BCF value: 165
The recommended BCF value was calculated using the geometric mean of 6 laboratory values as follows:			

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values	Reference	Experimental Parameters	Species
1,230	Freitag, Geyer, Kraus, Viswanathan, Kotzias, Attar, Klein, and Korte (1982)	3-day exposure duration	*Leuciscus idus*
448	Lu and Metcalf (1975)	Not reported. The values reported in Lu and Metcalf (1975) were converted to wet weight using an unit conversion factor of 5.0 [a]	*Gambusia affinis*
100 1,148	Podowski and Khan (1984)	16-day exposure duration	*Carassius auratus*
11	Spehar, Veith, DeFoe, and Bergstedt (1979)	30-day exposure duration	*Pimephales promelas*
29	Veith, DeFoe, and Bergstedt (1979)	32-day exposure duration	*Pimephales promelas*
Compound: Pentachlorobenzene			Recommended BCF value: 12,690
The recommended BCF value was calculated using the geometric mean of 12 laboratory values as follows:			
5,100 7,100 7,300	Banerjee, Suggatt, and O'Grady (1984)	2-day exposure duration	*Lepomis macrochirus* *Oncorynchus mykiss* *Poecilia reticulata*
26,000	Bruggeman, Oppenhuizen, Wijbenga, and Hutzinger (1984)	Not reported	*Poecilia reticulata*
8,400	Carlson and Kosian (1987)	31-day exposure duration	*Pimephales promelas*
28,183	Ikemoto, Motoba, Suzuki, Uchida (1992)	24-hour exposure duration	*Oryzias latipes*
260,000	Konemann and van Leeuwen (1980)	Not reported	*Poecilia reticulata*
17,000	Opperhuizen, Velde, Gobas, Liem, and Steen (1985)	Multiple exposure durations	*Poecilia reticulata*
6,600	Qiao and Farrell (1996)	10-day exposure duration	*Oncorhynchus mykiss*
23,000	Schrap and Opperhuizen (1990)	Not reported	*Poecilia reticulata*
4,700	Van Hoogen and Opperhuizen (1988)	5-day exposure duration; 21-day depuration	*Poecilia reticulata*
3,400	Veith, Macek, Petrocelli, and Carroll (1980)	28-day exposure duration	*Lepomis macrochirus*

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values	Reference	Experimental Parameters	Species
Compound: Pentachlorophenol			Recommended BCF value: 109
The recommended BCF value was calculated using the geometric mean of 20 laboratory values as follows:			
128 776	Garten and Trabalka (1983)	Not reported	Fish
189.5	Gates and Tjeerdema (1993)	1-day exposure duration	*Morone saxatilis*
2 131	Kobayashi and Kishino (1980)	1-hour exposure duration	*Carassius auratus*
350	Korte, Freitag, Geyer, Klein, Karus, and Lahaniatis (1978)	1-day exposure duration	*Zeucisens idus melanotus*
16 48 5 27	Parrish, Dyar, Enos, and Wilson (1978)	28 to 151-day exposure duration	*Cyprinodon variegatus*
30 38	Schimmel, Patrick, and Faas (1978)	28-day exposure duration	*Funidulus similis* *Mugil cephalus*
216	Smith, Bharath, Mallard, Orr, McCarty, and Ozburn (1990)	28-day exposure; 14-day depuration	*Jordanella floridae*
1,066 434 426 281	Spehar , Nelson, Swanson, and Renoos (1985)	32-day exposure duration	*Pimephales promelas*
52.3 607	Stehly and Hayton (1990)	96-hour exposure	*Carassius auratus*
770	Veith, DeFoe, and Bergstedt (1979)	32-day exposure	*Pimephales promelas*
Pesticides			
Compound: 4,4-DDE			Recommended BCF value: 25,512

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values	Reference	Experimental Parameters	Species
The recommended BCF value was calculated using the geometric mean of 11 laboratory values as follows:			
12,037	Metcalf, Sanborn, Lu, and Nye (1975)	Not reported	Fish
51,285 27,542	Garten and Trabalka (1983)	Freshwater	Fish
5,010 110,000 106,000 181,000	Hamelink and Waybrant (1976)	Not reported	*Lepomis macrochirus* *Oncorhynchus mykiss*
27,358	Metcalf, Sangha, and Kapoor (1971)	33-day exposure duration	*Gambusia affinis*
217 27,358	Metcalf, Kapoor, Lu, Schuth, and Sherman (1973)	3 to 33-day exposure duration	*Gambusia affinis*
81,000	Oliver and Niimi (1985)	96-day exposure duration	*Oncorhynchus mykiss*
51,000	Veith, DeFoe, and Bergstedt (1979)	32-day exposure duration	*Pimephales promelas*
Compound: Heptachlor			Recommended BCF value: 5,522
The recommended BCF value was calculated using the geometric mean of 7 laboratory values as follows:			
3,700 2,400 4,600	Goodman, Hansen, Couch, and Forester (1978)	28-day exposure duration	*Cyprinodon variegatus*
3,600 10,000	Schimmel, Patrick, and Forester (1976)	96-hour exposure duration	*Leiostomus xanthurus*
11,200	U.S. EPA (1980a)	Not reported	Fish
9,500	Veith, DeFoe, and Bergstedt (1979)	32-day exposure duration	*Pimephales promelas*
Compound: Hexachlorophene			Recommended BCF value: 278
The recommended BCF value was based on data from one study as follows:			
278	Sanborn (1974)	Not reported	*Oncorhychus mykiss*

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values	Reference	Experimental Parameters	Species
Inorganics			
Compound: Aluminum			Recommended BCF value: 2.70
The recommended BCF value was calculated using the geometric mean of 7 laboratory values as follows:			
0.05 1.25 0.05 0.35	Cleveland, Little, Hamilton, Buckler, and Hunn (1986)	37-day exposure duration	*Salvelinus fontinalis*
36 123 215	Cleveland, Buckler, and Brumbaugh (1991)	56-day exposure duration; 28-day depuration	*Salvelinus fontinalis*
Compound: Antimony			Recommended BCF value: 40
The recommended BCF value was based on one study as follows:			
40	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Fish
Compound: Arsenic			Recommended BCF value: 114
The recommended BCF value was calculated using the geometric mean of 3 laboratory values as follows:			
333 100	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Fish
44	U.S. EPA (1992b)	Not reported	Fish
Compound: Barium			Recommended BCF value: 633
Empirical data for this compound were not available. The recommended BCF is the arithmetic mean of the recommended values for 14 inorganics with empirical data available (aluminum, antimony, arsenic, beryllium, cadmium, chromium, copper, lead, mercury, nickel, selenium, silver, thallium, and zinc).			
Compound: Beryllium			Recommended BCF value: 62
The recommended BCF value was calculated using the geometric mean of 4 laboratory values as follows:			

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

(Page 14 of 19)

Reported Values	Reference	Experimental Parameters	Species
200 200	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Fish
19	U.S. EPA (1992b)	Not reported	Fish
19	U.S. EPA (1978)	28-day exposure duration	Fish
Compound: Cadmium			Recommended BCF value: 907
The recommended BCF value was calculated using the geometric mean of 4 field values.			
558 1,295 729 1,286	Saiki, Castleberry, May, Martin, and Ballard (1995)	Field samples. The field values reported in Saiki, Castleberry, May, Martin, and Ballard (1995) were converted to wet weight using a conversion factor of 5.0[a]. The field values are also based on mean values calculated for each of the 4 fish species.	*Catostomus occidentalis* *Gasterosteus aculeatus* *Ptychocheilus grandis* *Oncorhynchus tshawytasch*
716	Benoit, Leonard, Christensen, and Fiandt (1976)	38-week exposure duration; based on mean values calculated from various tissue concentrations in the kidney, liver, spleen, gonad, gills, and muscle/red blood cells. A unit conversion of 1,000 was applied to the value.	*Salvelinus fontanilis*
480	Eisler, Zaroogian, and Hennekey (1972)	3-week exposure duration	*Fundulus heteroclitus*
161 51	Harrison and Klaverkamp (1989)	72-day exposure duration, 25 and 63-day depuration	*Oncorhynchus mykiss* *Coregonus clupeatormis*
33	Kumada, Kimura, and Yokote (1980)	10 week exposure duration	*Oncorhynchus mykiss*
8 3,333	Kumada, Kimura, Yokote, and Matida (1973)	280-day exposure; values are based on a high to low range of values. The values reported in Kumada, Kimura, Yokote, and Matida (1973) were converted to wet weight using a conversion factor of 5.0[a].	*Oncorhynchus mykiss*
4.4	Spehar (1976)	30-day exposure duration	*Jordanella floridae*
3,000 200	Thompson, Burton, Quinn and Ng (1972)	Not reported	Fish

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

(Page 15 of 19)

Reported Values	Reference	Experimental Parameters	Species
4,100	Williams and Giesy (1979)	56-day exposure duration	Fish
Compound: Chromium (total)			Recommended BCF value: 19
The recommended BCF value was calculated using the geometric mean of 4 laboratory values as follows:			
1.27 1.34	Fromm and Stokes (1962)	30-day exposure duration; values are based on a high to low range of reported values.	*Oncorhynchus mykiss*
200 400	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Fish
Compound: Copper			Recommended BCF value: 710
The recommended BCF value was calculated using the geometric mean of 4 field values as follows:			
761 697 1,236 387	Saiki, Castleberry, May, Martin, and Ballard (1995)	Field samples	*Catostomus occidentalis* *Gasterosteus aculeatus* *Ptychocheilus grandis* *Oncorhynchus tshawytasch*
50 500 667	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Fish
36	U.S. EPA (1992b)	Not reported	Fish

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values	Reference	Experimental Parameters	Species
Compound: Cyanide (total)			Recommended BCF value: 633
Empirical data for this compound were not available. The recommended BCF is the arithmetic mean of the recommended values for 14 inorganics with empirical data available (aluminum, antimony, arsenic, beryllium, cadmium, chromium, copper, lead, mercury, nickel, selenium, silver, thallium, and zinc).			
Compound: Lead			Recommended BCF value: 0.09
The recommended BCF value based on one field value:			
0.09	Atchinson, Murphy, Bishop, McIntosh, and Mayes (1977)	Field samples. The values reported in Atchinson, Murphy, Bishop, McIntosh, and Mayes (1977) were converted to wet weight using a conversion factor of 5.0[a].	*Lepomis macrochiras*
0.15 0.17	Holcombe, Benoit, Leonard, and McKim (1976)	266-day exposure duration. The values reported in Holcombe, Benoit, Leonard, and McKim (1976) were converted to wet weight using a conversion factor of 5.0[a]. Mean values were calculated based on tissue concentrations in the red blood cells, kidney, and muscle.	*Salvelinus fontanilis*
300 100	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Fish
Compound: Mercuric chloride			Recommended BCF value: 3,530
The recommended BCF value was calculated using the geometric mean of 3 laboratory values as follows:			
1,800	Boudou and Ribeyre (1984)	60-day exposure duration	*Oncorhynchus mykiss*
4,380 5,580	Snarski and Olson (1982)	287-day exposure duration; values are based on a high to low range of reported values.	*Pimephales promelas*
Compound: Methyl mercury			Recommended BCF value: 11,168
The recommended BCF value was calculated using the geometric mean of 3 laboratory values as follows:			
11,000	Boudou and Ribeyre (1984)	60-day exposure duration	*Oncorhynchus mykiss*

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values	Reference	Experimental Parameters	Species
10,800 11,724	McKim, Olson, Holcome, and Hunt (1976)	756-day exposure duration	*Salvelinus fontinalis*
Compound: Nickel			Recommended BCF value: 78
The recommended BCF value was calculated using the geometric mean of 3 laboratory values as follows:			
100 100	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Fish
47	U.S. EPA (1992b)	Not reported	Fish
Compound: Selenium			Recommended BCF value: 129
The recommended BCF value was calculated using the geometric mean of 12 laboratory values as follows:			
18	Adams (1976)	96-day exposure duration	Fish
4,900	Besser, Canfield, and LaPoint (1993)	30-day exposure duration	*Lepomis reinhardtii*
5 7	Cleveland , Little, Buckler, and Wiedmeyer (1993)	60-day exposure duration; values are based on a high to low range of reported values.	*Lepomis macrochirus*
154 711	Dobbs, Cherry, and Cairns (1996)	25-day exposure duration	*Pimephales promelas*
3 240	Hodson, Spry, and Blunt (1980)	351-day exposure duration; values represent a high to low range of reported values based on BCFs for peritoneal fat and the liver.	*Oncorhynchus mykiss*
285 465	Lemly (1982)	120-day exposure duration	*Micropterus salmoides* *Lepomis macrochirus*
4,000 167	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Fish
Compound: Silver			Recommended BCF value: 87.71
The recommended BCF value was calculated using the geometric mean of 2 laboratory values as follows:			
3,330	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Fish

TABLE C-5

WATER-TO-FISH BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg dissolved COPC / L water)

Reported Values	Reference	Experimental Parameters	Species
Compound: Thallium			Recommended BCF value: 10,000
The recommended BCF value was calculated using the geometric mean of 2 laboratory values as follows:			
10,000 10,000	Thompson, Burton, Quinn, and Ng (1972)	Not reported	Fish
Compound: Zinc			Recommended BCF value: 2,059
The recommended BCF value was calculated using the geometric mean of 4 field values as follows:			
2,299 2,265 4,290 804	Saiki, Castleberry, May, Martin, and Ballard (1995)	Field samples.	*Catostomus occidentalis* *Gasteroteus aculeatus* *Ptychocheilus grandis* *Oncorhynchus tshawytasch*
50 130 130 200	Deutch, Borg, Kloster, Meyer, and Moller (1980)	9-day exposure duration	*Spinachia vulgaris* *Gasterosteus acul.* *Pungitius pungitius* *Cottus scorpius*
373 8,853	Pentreath (1973)	180-day exposure duration; values are based on a high to low range of reported values	*Pleuronectes platessa*
1,000 2,000 2,000	Thompson, Burton, Quinn and Ng (1972)	Not reported	Fish
47	U.S. EPA (1992b)	Not reported	Fish

Notes:

(a) The reported values are presented as the amount of COPC in fish tissue divided by the amount of COPC in water. If the values reported in the studies were presented as dry tissue weight, they were converted to wet weight by dividing the concentration in dry fish tissue weight by 5.0. This conversion factor assumes a fish's total weight is 80.0 percent moisture (Holcomb, Benoit, Leonard, and McKim 1976).

The conversion factor was calculated as follows:

$$Conversion\ factor = \frac{1.0\ g\ fish\ total\ weight}{1.0\ g\ fish\ total\ weight - 0.80\ g\ fish\ wet\ weight}$$

(b) The equation used to convert the total organic COPC concentrations in field samples to dissolved COPC concentrations is from U.S. EPA (1995a) as follows:

$BAF\ (dissolved) = (BAF\ (total) / f_{fd}) - 1$

where: *BAF (dissolved)* = *BAF* based on dissolved concentration of COPC in water
BAF (total) = *BAF* based on the field derived data for total concentration of COPC in water
f_{fd} = Fraction of COPC that is freely dissolved in the water
where: $f_{fd} = 1 / [1 + ((DOC \times K_{ow}) / 10) + (POC \times K_{ow})]$
DOC = Dissolved organic carbon, Kg of organic carbon / L of water (2.0×10^{-06} kg/L)
K_{ow} = Octanol-water partition coefficient of the COPC, as reported in U.S. EPA (1994b)
POC = Particulate organic carbon, Kg of organic carbon / L of water (7.5×10^{-09} Kg/L)

(c) The reported field *BAF*s were converted to *BCF*s as follows:

$BCF = (BAF_{TLn} / FCM_{TLn}) - 1$

where: BAF_{TLn} = The reported field bioaccumulation factor for the trophic level "n" of the study species.
FCM_{TLn} = The food chain multiplier for the trophic level "n" of the study species.

(d) PCB values were converted to dissolved COPC BCFs based on the K_{ow} for Aroclor 1254.

(e) The geometric mean of the converted field derived BCFs was compared to the geometric mean of the laboratory derived BCFs. The higher of the two values was selected as the COPC BCF.

TABLE C-6

SEDIMENT-TO-BENTHIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg COPC / kg dry sediment)

Reported Values[a]	Reference	Experimental Parameters	Species
Dioxins and Furans			
Compound: 2,3,7,8-Tetrachlorodibenzo-p-dioxin (2,3,7,8-TCDD)			Recommended BCF value: 19,596
Empirical data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 6.64 (U.S. EPA 1994a)			
Compound: 1,2,3,7,8-Pentachlorodibenzo(p)dioxin (1,2,3,7,8-PeCDD)			Recommended BCF value: 18,023
The BCF was calculated using the TCDD BCF and a congener-speccific bioaccumulation equivalency factor (BEF) (U.S. EPA 1995b) as follows: BCF =19,596 x 0.92 = 3,896			
Compound: 1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin (1,2,3,4,7,8-HxCDD)			Recommended BCF value: 6,075
The BCF was calculated using the TCDD BCF and a congener-specific BEF (U.S. EPA 1995b) as follows: BCF =19,596 x 0.31 =1313			
Compound: 1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin (1,2,3,6,7,8-HxCDD)			Recommended BCF value: 2,351
The BCF was calculated using the TCDD BCF and a congener-specific BEF (U.S. EPA 1995b) as follows: BCF =19,596 x 0.12 =2,351			
Compound: 1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin (1,2,3,7,8,9-HxCDD)			Recommended BCF value: 2,743
The BCF was calculated using the TCDD BCF and a congener-specific BEF (U.S. EPA 1995b) as follows: BCF =19,596 x 0.14 =2,743			
Compound: 1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin (1,2,3,4,6,7,8-HpCDD)			Recommended BCF value: 99.4
The BCF was calculated using the TCDD BCF and a congener-specific BEF (U.S. EPA 1995b) as follows: BCF =19,596 x 0.051 =99.4			
Compound: Octachlorodibenzo-p-dioxin (OCDD)			Recommended BCF value: 23.5
The BCF was calculated using the TCDD BCF and a congener-specific BEF (U.S. EPA 1995b) as follows: BCF =19,596 x 0.012 =23.5			
Compound: 2,3,7,8-Tetrachlorodibenzofuran (2,3,7,8-TCDF)			Recommended BCF value: 2,642
The BCF was calculated using the TCDD BCF and a congener-specific BEF (U.S. EPA 1995b) as follows: BCF = 3,302 x0.80 = 2,642			
Compound: 1,2,3,7,8-Pentachlorodibenzo-p-furan (1,2,3,7,8-PeCDF)			Recommended BCF value: 4,311
The BCF was calculated using the TCDD BCF and a congener-specific BEF (U.S. EPA 1995b) as follows: BCF =19,596 x 0.22 =4,311			
Compound: 2,3,4,7,8-Pentachlorodibenzo-p-furan (2,3,4,7,8-PeCDF)			Recommended BCF value: 31,354
The BCF was calculated using the TCDD BCF and a congener-specific BEF (U.S. EPA 1995b) as follows: BCF =19,596 x 1.6 =31,354			

TABLE C-6

SEDIMENT-TO-BENTHIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg COPC / kg dry sediment)

Reported Values[a]	Reference	Experimental Parameters	Species
Compound: 1,2,3,4,7,8-Hexachlorodibenzo-p-furan (1,2,3,4,7,8-HxCDF)			Recommended BCF value: 1,489
The BCF was calculated using the TCDD BCF and a congener-specific BEF (U.S. EPA 1995b) as follows: BCF =19,596 x 0.076 =1,489			
Compound: 1,2,3,6,7,8-Hexachlorodibenzo-p-furan (1,2,3,6,7,8-HxCDF)			Recommended BCF value: 3,723
The BCF was calculated using the TCDD BCF and a congener-specific BEF (U.S. EPA 1995b) as follows: BCF =19,596 x 0.19 =3,723			
Compound: 2,3,4,6,7,8-Hexachlorodibenzo-p-furan (2,3,4,6,7,8-HxCDF)			Recommended BCF value: 13,129
The BCF was calculated using the TCDD BCF and a congener-specific BEF (U.S. EPA 1995b) as follows: BCF =19,596 x 0.67 = 13,129			
Compound: 1,2,3,7,8,9-Hexachlorodibenzo-p-furan (1,2,3,7,8,9-HxCDF)			Recommended BCF value: 12,345
The BCF was calculated using the TCDD BCF and a congener-specific BEF (U.S. EPA 1995b) as follows: BCF =19,596 x 0.63 =12,345			
Compound: 1,2,3,4,6,7,8,-Heptachlorodibenzo-p-furan (1,2,3,4,6,7,8-HpCDF)			Recommended BCF value: 215.6
The BCF was calculated using the TCDD BCF and a congener-specific BEF (U.S. EPA 1995b) as follows: BCF =19,596 x 0.011 =215.6			
Compound: 1,2,3,4,7,8,9-Heptachlorodibenzo-p-furan (1,2,3,4,7,8,9-HpCDF)			Recommended BCF value: 7,642
The BCF was calculated using the TCDD BCF and a congener-specific (U.S. EPA 1995b) as follows: BCF =19,596 x 0.39 =7,642			
Compound: Octachlorodibenzo-p-furan (OCDF)			Recommended BCF value: 313.5
The BCF was calculated using the TCDD BCF and a congener-specific BEF (U.S. EPA 1995b) as follows: BCF =19,596 x 0.016 =313.5			
Polynuclear Aromatic Hydrocarbons (PAHs)			
Compound: Benzo(a)pyrene			Recommended BCF value: 1. 59
The recommended BCF value was calculated using the geometric mean of 8 values as follows:			
5.2 2.8	Augenfeld, Anderson, Riley, and Thomas (1982)	60-day exposure duration	*Macoma inquinata* *Abarenicola pacifica*
0.4 0.65 7.4	Driscoll and McElroy (1996)	6 to 12-day exposure duration	*Nereis diversicolor* *Scolecolipides virdis* *Leitoscoloplos fragilis*

TABLE C-6

SEDIMENT-TO-BENTHIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg COPC / kg dry sediment)

Reported Values[a]	Reference	Experimental Parameters	Species
2.3 6.9	Landrum, Eadie, and Faust (1991)	Mixture of PAH at four concentrations	*Diporeia* sp.
0.09	Roesijadi, Anderson, and Blaylock (1978)	7-day exposure duration	*Macoma inquinata*
Compound: Benzo(a)anthracene			Recommended BCF value: 1.45
Empirical data for this compound were not available. Therefore, the BCF for benzo(a)pyrene was used as a surrogate.			
Compound: Benzo(b)fluoranthene			Recommended BCF value: 1.61
Empirical data for this compound were not available. Therefore, the BCF for benzo(a)pyrene was used as a surrogate.			
Compound: Benzo(k)fluoranthene			Recommended BCF value: 1.61
Empirical data for this compound were not available. Therefore, the BCF for benzo(a)pyrene was used as a surrogate.			
Compound: Chrysene			Recommended BCF value: 1.38
BCF value was calculated using the geometric mean of 3 values as follows:			
0.04	Roesijadi, Anderson, and Blaylock (1978)	7-day exposure duration	*Macoma inquinata*
11.6 5.64	Augenfeld, Anderson, Riley, and Thomas (1982)	60-day exposure duration	*Macoma inquinata* *Abarenicola pacifica*
Compound: Dibenz(a,h)anthracene			Recommended BCF value: 1.61
Empirical data for this compound were not available. Therefore, the BCF for benzo(a)pyrene was used as a surrogate.			
Compound: Indeno(1,2,3-cd)pyrene			Recommended BCF value: 1.61
Empirical data for this compound were not available. Therefore, the BCF for benzo(a)pyrene was used as a surrogate.			
Polychlorinated Biphenyls (PCBs)			
Compound: Aroclor 1016			Recommended BCF value: 0.53
The recommended BCF value was calculated using the geometric mean of 2 empirical values as follows:			

TABLE C-6

SEDIMENT-TO-BENTHIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg COPC / kg dry sediment)

Reported Values[a]	Reference	Experimental Parameters	Species
0.2 1.4	Wood, O'Keefe, and Bush (1997)	12-day exposure duration; 1-day depuration	*Chironomus tentans*
Compound: Aroclor 1254			Recommended BCF value: 0.53
The recommended BCF value was calculated using the geometric mean of 2 empirical values as follows:			
0.2 1.4	Wood, O'Keefe, and Bush (1997)	12-day exposure duration; 1-day depuration	*Chironomus tentans*
Nitroaromatics			
Compound: 1,3-Dinitrobenzene			Recommended BCF value: 1.19
Empirical data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 1.491 (U.S. EPA 1994b)			
Compound: 2,4-Dinitrotoluene			Recommended BCF value: 58
The recommended BCF value was based on 1 study as follows:			
58	Liu, Bailey, and Pearson (1983)	4-day exposure duration	*Lumbriculus variegatus*
Compound: 2,6-Dinitrotoluene			Recommended BCF value: 2.50
Empirical data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 1.886 (U.S. EPA 1994b)			
Compound: Nitrobenzene			Recommended BCF value: 2.27
Empirical data were not available for this compound. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 1.833 (U.S. EPA 1994b)			
Compound: Pentachloronitrobenzene			Recommended BCF value: 451
Empirical data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 4.640 (U.S. EPA 1994b)			
Phthalate Esters			
Compound: Bis(2-ethylhexyl)phthalate			Recommended BCF value: 1,309

TABLE C-6

SEDIMENT-TO-BENTHIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg COPC / kg dry sediment)

Reported Values[a]	Reference	Experimental Parameters	Species
Empirical data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 5.205 (U.S. EPA 1994b)			
Compound: Di(n)octyl phthalate			Recommended BCF value: 3,128,023
Empirical data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 9.330 (U.S. EPA 1994b)			
Volatile Organic Compounds			
Compound: Acetone			Recommended BCF value: 0.05
Empirical data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = -0.222 (Karickoff and Long 1995)			
Compound: Acrylonitrile			Recommended BCF value: 0.11
Empirical data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 0.250 (Karickoff and Long 1995)			
Compound: Chloroform			Recommended BCF value: 2.82
Empirical data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 1.949 (U.S. EPA 1994b)			
Compound: Crotonaldehyde			Recommended BCF value: 0.20
Empirical data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 0.55 (based on equations developed by Hansch and Leo 1979, as calculated in NRC 1981)			
Compound: 1,4-Dioxane			Recommended BCF value: 0.04
Empirical data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = -0.268 (U.S. EPA 1995a)			
Compound: Formaldehyde			Recommended BCF value: 0.14
Empirical data for this compound were not available.The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 0.342 (U.S. EPA 1995a)			
Compound: Vinyl chloride			Recommended BCF value: 0.62

TABLE C-6

SEDIMENT-TO-BENTHIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg COPC / kg dry sediment)

Reported Values[a]	Reference	Experimental Parameters	Species
Empirical data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 1.146 (U.S. EPA 1994b)			
Other Chlorinated Organics			
Compound: Carbon tetrachloride			Recommended BCF value: 12
Empirical data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 2.717 (U.S. EPA 1994b)			
Compound: Hexachlorobenzene			Recommended BCF value: 2,296
Empirical data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 5.503 (U.S. EPA 1994b)			
Compound: Hexachlorobutadiene			Recommended BCF value: 0.44
The recommended BCF value was based on empirical data from one study as follows:			
0.44	Oliver (1987)	79-day exposure duration; The values reported in Oliver (1987) were converted to wet weight over dry weight using a conversion factor of 5.99[a].	Oligochaetes
Compound: Hexachlorocyclopentadiene			Recommended BCF value: 746
Empirical data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 4.907 (U.S. EPA 1994b)			
Compound: Pentachlorobenzene			Recommended BCF value: 0.32
The recommended BCF value is based on 1 study as follows:			
0.32	Oliver (1987)	79-day exposure duration; The values reported in Oliver (1987) were converted to wet weight over dry weight using a conversion factor of 5.99[a].	Oligochaetes
Compound: Pentachlorophenol			Recommended BCF value: 1,034
Empirical data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 5.080 (U.S. EPA 1994b)			

TABLE C-6

SEDIMENT-TO-BENTHIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg COPC / kg dry sediment)

Reported Values[a]	Reference	Experimental Parameters	Species
Pesticides			
Compound: 4,4'-DDE			Recommended BCF value: 0.95
The recommended BCF value was calculated using the geometric mean of 13 values as follows:			
2.9 1.3 0.4 0.2 2.2 0.1 1.2 9.6 2.1 24.6 1.8 0.1 0.07	Reich, Perkins, and Cutter (1986)	Field samples	Tubificidae Chironomidae Croixidae
Compound: Heptachlor			Recommended BCF value: 1.67
Empirical data for heptachlor were not available. The BCF was calculated from 1 field-derived value for heptachlor epoxide as follows:			
10.0	Beyer and Gish (1980)	Field samples; The value reported in Beyer and Gish (1980) was converted to wet weight over dry weight using a conversion factor of 5.99[a].	*Aporrectodea trapezoides* *Aparrectodea turgida* *Allolobophora chlorotica* *Lumbricus terrestris*
Compound: Hexachlorophene			Recommended BCF value: 106,970
Empirical data for this compound were not available. The BCF was calculated using the following regression equation: log BCF = 0.819 x log K_{ow} - 1.146 (Southworth, Beauchamp, and Schmieder 1978), where log K_{ow} = 7.540 (Karickoff and Long 1995)			
Inorganics			
Compound: Aluminum			Recommended BCF value: 0.90
Empirical data for this compound were not available. The recommended BCF value is the arithmetic average of 6 recommended values for those metals with empirical data (cadmium, chromium, copper, lead, inorganic mercury, and zinc).			
Compound: Antimony			Recommended BCF value: 0.90
Empirical data for this compound were not available. The recommended BCF value is the arithmetic average of 6 recommended values for those metals with empirical data (cadmium, chromium, copper, lead, inorganic mercury, and zinc).			

TABLE C-6

SEDIMENT-TO-BENTHIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg COPC / kg dry sediment)

Reported Values[a]	Reference	Experimental Parameters	Species
Compound: Arsenic			Recommended BCF value: 0.90
Empirical data for this compound were not available. The recommended BCF value is the arithmetic average of 6 recommended values for those metals with empirical data (cadmium, chromium, copper, lead, inorganic mercury, and zinc).			
Compound: Barium			Recommended BCF value: 0.90
Empirical data for this compound were not available. The recommended BCF value is the arithmetic average of 6 recommended values for those metals with empirical data (cadmium, chromium, copper, lead, inorganic mercury, and zinc).			
Compound: Beryllium			Recommended BCF value: 0.90
Empirical data for this compound were not available. The recommended BCF value is the arithmetic average of 6 recommended values for those metals with empirical data (cadmium, chromium, copper, lead, inorganic mercury, and zinc).			
Compound: Cadmium			Recommended BCF value: 3.4
The recommended BCF value was calculated using the geometric mean of 8 field-derived values as follows:			
3.33 7.68 1.79 7.15 1.67 2.34 2.27 6.29	Saiki, Castleberry, May, Martin, and Bullard (1995)	Field samples; The values reported in Saiki, Castleberry, May, Martin, and Bullard (1995) were converted to wet weight over dry weight using a conversion factor of 5.99[a].	Chironomidae Epheroptera
Compound: Chromium (total)			Recommended BCF value: 0.39
The recommended BCF value was based on 1 field-derived value as follows:			
0.39	Namminga and Wilhm (1977)	Field samples	Chironomidae
0.03 0.07 0.001 0.003	Capuzzo and Sasner (1977)	168-day exposure duration; The reported value was calculated by dividing the tissue concentration by the media concentration [(µg/g)/(mg/g)] and a conversion factor of $1x10^{-3}$ was applied to the value. A conversion factor of 5.99[a] was applied to convert dry tissue weight to wet weight.	*Mya arenaria*
Compound: Copper			Recommended BCF value: 0.30

TABLE C-6

SEDIMENT-TO-BENTHIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg COPC / kg dry sediment)

Reported Values[a]	Reference	Experimental Parameters	Species
The recommended BCF value was calculated using the geometric mean of 9 field values as follows:			
0.11 0.22 0.13 0.32	Jones, Jones, and Radlett (1976)	25-day exposure duration; The values reported in Jones, Jones, and Radlett (1976) were converted to wet weight over dry weight using a conversion factor of 5.99[a].	*Nereis diveriscolor*
1.1	Namminga and Wilhm (1977)	Field samples	Chironomidae
0.29 0.36 0.16 0.73 0.31 0.36 0.06 0.25	Saiki, Castleberry, May, Martin and Bullard (1995)	Field samples; The values reported in Saiki, Castleberry, May, Martin and Bullard (1995) were converted to wet weight over dry weight using a conversion factor of 5.99[a].	Chironomidae Ephemeroptera
Compound: Cyanide (total)			Recommended BCF value: 0.90
Empirical data were not available for this compound. The recommended BCF value is the arithmetic average of 6 recommended values for those metals with empirical data (cadmium, chromium, copper, lead, inorganic mercury, and zinc).			
Compound: Lead			Recommended BCF value: 0.63
The recommended BCF value was based on 1 study follows:			
0.4 1.0	Harrahy and Clements (1997)	14-day exposure duration	*Chironomus tentans*
Compound: Mercuric chloride			Recommended BCF value: 0.068
The recommended BCF value was based on 6 field values as follows:			
0.08	Saouter, Hare, Campbell, Boudou, and Ribeyre (1993)	9-day exposure duration	*Hexagenia rigida*
0.16 0.08 0.04 0.04 0.08 0.06	Hildebrand, Strand, and Huckabee (1980)	Field samples	Hydropsychidae, Corydalus, Decapoda, Aterix, Psephenidae, and unspecified other benthic invertebrates
Compound: Methyl mercury			Recommended BCF value: 0.48
The recommended BCF value was based on 6 field values as follows:			

TABLE C-6

SEDIMENT-TO-BENTHIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg COPC / kg dry sediment)

Reported Values[a]	Reference	Experimental Parameters	Species
4.0	Saouter, Hare, Campbell, Boudou, and Ribeyre (1993)	9-day exposure duration	*Hexagenia rigida*
1.45 0.50 0.26 0.41 0.37 0.44	Hildebrand, Strand, and Huckabee (1980)	Field samples	Hydropsychidae, Corydalus, Decapoda, Aterix, Psephenidae, and unspecified other benthic invertebrates
Compound: Nickel			Recommended BCF value: 0.90
Empirical data for this compound were not available. The recommended BCF value is the arithmetic average of 6 recommended values for those metals with empirical data (cadmium, chromium, copper, lead, inorganic mercury, and zinc).			
Compound: Selenium			Recommended BCF value: 0.90
Empirical data for this compound were not available. The recommended BCF value is the arithmetic average of 6 recommended values for those metals with empirical data (cadmium, chromium, copper, lead, inorganic mercury, and zinc).			
Compound: Silver			Recommended BCF value: 0.90
Empirical data for this compound were not available. The recommended BCF value is the arithmetic average of 6 recommended values for those metals with empirical data (cadmium, chromium, copper, lead, inorganic mercury, and zinc).			
Compound: Thallium			Recommended BCF value: 0.90
Empirical data for this compound were not available. The recommended BCF value is the arithmetic average of 6 recommended values for those metals with empirical data (cadmium, chromium, copper, lead, inorganic mercury, and zinc).			
Compound: Zinc			Recommended BCF value: 0.57
The recommended BCF value was calculated using the geometric mean of 8 field values as follows:			
3.6	Namminga and Wilhm (1977)	Not reported	Chironomidae
0.46 0.38 0.13 0.79 0.83 1.16 0.39 1.57	Saiki, Castleberry, May, Martin, and Bullard (1995)	Field samples; the values reported in Saiki, Castleberry, May, Martin and Bullard (1995) were converted to wet weight over dry weight using an unit conversion factor of 5.99[a].	Chironomidae Ephemeroptera

TABLE C-6

SEDIMENT-TO-BENTHIC INVERTEBRATE BIOCONCENTRATION FACTORS
(mg COPC / kg wet tissue) / (mg COPC / kg dry sediment)

Notes:

(a) The reported values are presented as the amount of compound in invertebrate tissue divided by the amount of compound in the sediment. If the values reported in the studies were presented as dry tissue weight over dry sediment weight, they were converted to wet weight over dry weight by dividing the concentration in dry invertebrate tissue weight by 5.99. This conversion factor assumes an earthworm's total weight is 83.3 percent moisture (Pietz et al. 1984).

The conversion factor was calculated as follows:

$$Conversion\ factor = \frac{1.0\ g\ invertebrate\ total\ weight}{1.0\ g\ invertebrate\ total\ weight - 0.833\ g\ invertebrate\ wet\ weight}$$

TABLE C-7

AIR-TO-PLANT BIOTRANSFER FACTORS
(µg COPC / g dry plant) / (µg COPC / g air)

(Page 1 of 3)

Compound	*Bv* Value[a]	Compound	*Bv* Value
Dioxins and furans			
2,3,7,8-Tetrachlorodibenzo-p-dioxin (2,3,7,8-TCDD)	6.55E+04	1,2,3,7,8-Pentachlorodibenzo-p-furan (1,2,3,7,8-PeCDF)	9.75E+04
1,2,3,7,8-Pentachlorodibenzo(p)dioxin (1,2,3,7,8-PeCDD)	2.39E+05	2,3,4,7,8-Pentachlorodibenzo-p-furan (2,3,4,7,8-PeCDF)	9.75E+04
1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin (1,2,3,4,7,8-HxCDD)	5.20E+05	1,2,3,4,7,8-Hexachlorodibenzo-p-furan (1,2,3,4,7,8-HxCDF)	1.62E+05
1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin (1,2,3,6,7,8-HxCDD)	5.20E+05	1,2,3,6,7,8-Hexachlorodibenzo-p-furan (1,2,3,6,7,8-HxCDF)	1.62E+05
1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin (1,2,3,7,8,9-HxCDD)	5.20E+05	2,3,4,6,7,8-Hexachlorodibenzo-p-furan (2,3,4,6,7,8-HxCDF)	1.62E+05
1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin (1,2,3,4,6,7,8-HpCDD)	9.10E+05	1,2,3,7,8,9-Hexachlorodibenzo-p-furan (1,2,3,7,8,9-HxCDF)	1.62E+05
Octachlorodibenzo-p-dioxin (OCDD)	2.36E+06	1,2,3,4,6,7,8,-Heptachlorodibenzo-p-furan (1,2,3,4,6,7,8-HpCDF)	8.30E+05
2,3,7,8-Tetrachlorodibenzofuran (2,3,7,8-TCDF)	4.57E+04	1,2,3,4,7,8,9-Heptachlorodibenzo-p-furan (1,2,3,4,7,8,9-HpCDF)	8.30E+05
Octachlorodibenzo-p-furan (OCDF)	2.28E+06		
Polynuclear aromatic hydrocarbons (PAHs)			
Benzo(a)pyrene	2.25E+05	Chrysene	5.97E+04
Benzo(a)anthracene	1.72E+04	Dibenzo(a,h)anthracene	4.68E+07
Benzo(b)fluoranthene	3.65E+04	Ideno(1,2,3-cd)pyrene	2.67E+08
Benzo(k)fluoranthene	5.40E+05		
Polychlorinated biphenyls (PCBs)			
Aroclor 1016	7.52E+01	Aroclor 1254	3.09E+02
Nitroaromatics			
1,3-Dinitrobenzene	1.74E+01	Nitrobenzene	2.43E-01
2,4-Dintrotoluene	5.10E+01	Pentachloronitrobenzene	1.71E-01

TABLE C-7

AIR-TO-PLANT BIOTRANSFER FACTORS
(µg COPC / g dry plant) / (µg COPC / g air)

Compound	*Bv* Value[a]	Compound	*Bv* Value
2,6-Dinitrotoluene	4.41E+01		
Phthalate esters			
Bis(2-ethylhexyl)phthalate	2.33E+03	Di(n)octyl phthalate	6.30E+08
Volatile organic compounds			
Acetone	1.13E-03	1,4-Dioxane	5.93E-03
Acrylonitrile	1.04E-03	Formaledehyde	4.65E-04
Chloroform	1.65E-03	Vinyl chloride	2.95E-06
Crotonaldehyde	Not Available		
Other chlorinated organics			
Carbon Tetrachloride	1.52E-03	Pentachlorphenol	1.02E+03
Hexachlorbenzene	7.57E+01	4,4'-DDE	2.08E+03
Hexachlorobutadiene	2.55E-01	Heptachlor	2.09E+03
Hexachlorocyclopentadiene	5.47E-01	Hexachlorophene	1.23E+10
Pentachlorobenzene	6.04E-01		
Inorganics			
Aluminum	0	Lead	0
Antimony	0	Mercuric chloride	1.80E+03
Arsenic	0	Methyl mercury	Not Applicable
Barium	0	Nickel	0
Beryllium	0	Selenium	0

TABLE C-7

AIR-TO-PLANT BIOTRANSFER FACTORS
(µg COPC / g dry plant) / (µg COPC / g air)

Compound	*Bv* Value[a]	Compound	*Bv* Value
Cadmium	0	Silver	0
Chromium (hexavalent)	0	Thallium	0
Copper	0	Zinc	0
Cyanide (total)	0		

Notes:

(a) The reported values were obtained from the references cited in Section C-1.7, and are consistent with the values provided in U.S. EPA (1998). Values for dioxin and furan congeners were obtained from the following:

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APPENDIX D

BIOCONCENTRATION FACTORS (*BCF*s) FOR WILDLIFE MEASUREMENT RECEPTORS

Screening Level Ecological Risk Assessment Protocol

August 1999

APPENDIX D

TABLE OF CONTENTS

Section **Page**

APPENDIX D

WILDLIFE MEASUREMENT RECEPTOR *BCF*s

Appendix D provides recommended guidance for determining values for compound-specific, media to receptor, bioconcentration factors (*BCF*s) for wildlife measurement receptors. Wildlife measurement receptor *BCF*s should be based on values reported in the scientific literature, or estimated using physical and chemical properties of the compound. Guidance on use of *BCF* values in the screening level ecological risk assessment is provided in Chapter 5.

Section D-1.0 provides the general guidance recommended to select or estimate compound *BCF* values for wildlife measurement receptors. Sections D-1.0 through D-1.3 further discuss determination of *BCF*s for specific media and receptors. References cited in Sections D-1.1 through D-1.3 are located following Section D-1.3.

For the compounds commonly identified in risk assessments for combustion facilities (identified in Chapter 2) and the mammal and bird example measurement receptors listed in Chapter 4, *BCF* values have been determined following the guidance in Sections D-1.0 through D-1.3. *BCF* values for these limited number of compounds and pathways are included in this appendix (see Tables D-1 through D-3) to facilitate the completion of screening ecological risk assessments. However, it is expected that *BCF* values for additional compounds and receptors may be required for evaluation on a site specific basis. In such cases, *BCF* values for these additional compounds could be determined following the same guidance (Sections D-1.0 through D-1.3) used in determination of the *BCF* values reported in this appendix. For the calculation of *BCF* values for measurement receptors not represented in Sections D-1.1 through D1-3 (e.g., amphibians and reptiles), an approach consistent to that presented in this appendix could be utilized by applying data applicable to those measurement receptors being evaluated.

For additional discussion on some of the references and equations cited in Sections D-1.0 through D-1.3, the reader is recommended to review the Human Health Risk Assessment Protocol (HHRAP) (U.S. EPA 1998) (see Appendix A-3), and the source documents cited in the reference section of this appendix.

D-1.0 GENERAL GUIDANCE

This section describes general procedures for developing compound-specific *BCF*s from biotransfer factors (*Ba*) for assessing exposure of measurement receptors. A biotransfer factor is the ratio of the compound concentration in fresh (wet) weight animal tissue to the daily intake of compound by the animal through ingestion of food items and media (soil, sediment, surface water). Therefore, as discussed in Chapter 5, biotransfer factors and receptor-specific ingestion rates can be used to calculate food item- and media-to-animal *BCF*s. This approach provides an estimate of biotransfer of compounds from applicable food items and media to measurement receptors ingesting these items.

Biotransfer factors could also be used directly in equations to calculate dose to measurement receptors. However, in order to promote consistency in evaluating exposure across all trophic levels within complex food webs, *BCF*s calculated from *Ba* values are recommended in this guidance for evaluating measurement receptors. The use of *Ba* values to determine *BCF* values, and the use of *BCF* values in general, for the estimation of compound concentrations in measurement receptors may introduce

uncertainty. Major factors that influence the uptake of a compound by an animal, and therefore uncertainty, include bioavailability, metabolic rate, type of digestive system, and feeding behavior. Uncertainties also should be considered regarding the development of biotransfer values in comparison to how they are being applied for estimating exposure. For example, biotransfer values may be used to estimate contaminant uptake to species from items ingested that differ from the species and intakes used to empirically develop the values. Also, biotransfer data reported in literature may be specific to tissue or organ analysis versus whole body. As a result, *BCF*s may be under- or over-estimated to an unknown degree.

BCFs for Measurement Receptors Ingesting Food Items *BCF* values for measurement receptors ingesting food items (plants or prey) can be calculated using the compound specific *Ba* value applicable to the animal (e.g., mammal, bird, etc.) and the measurement receptor-specific ingestion rate as follows:

$$BCF_{F\text{-}A} = Ba_A \cdot IR_F \qquad \text{Equation D-1-1}$$

where

$BCF_{F\text{-}A}$ = Bioconcentration factor for food item (plant or prey)-to-animal (measurement receptor) [(mg COPC/kg FW tissue)/(mg COPC/kg FW food item)]

Ba_A = COPC-specific biotransfer factor applicable for the animal (day/kg FW tissue)

IR_F = Measurement receptor food item ingestion rate (kg FW/day)

As an example of applying the above equation, *BCF* values for plants-to-wildlife measurement receptors listed in Chapter 4 are provided in Table D-1 at the end of this appendix. Measurement-receptor specific ingestion rates used to calculate *BCF*s are presented in Table 5-1. *Ba* values applicable to the mammal and bird measurement receptors in Table D-1 are discussed in Sections D-1.1 and D-1.2, respectively.

BCFs for Measurement Receptors Ingesting Media *BCF* values for measurement receptors in trophic levels 2, 3, and 4 ingesting media (i.e., soil, surface water, and sediment) can be calculated using the compound specific *Ba* value applicable to the animal (e.g., mammal, bird, etc.) and the measurement receptor-specific ingestion rate as follows:

$$BCF_{M\text{-}A} = Ba_A \cdot IR_M \qquad \text{Equation D-1-2}$$

where

$BCF_{M\text{-}A}$ = Bioconcentration factor for media-to-animal (measurement receptor) [(mg COPC/kg FW tissue)/(mg COPC/kg WW or DW media)]

Ba_A = COPC-specific biotransfer factor applicable for the animal (day/kg FW tissue)

IR_M = Measurement receptor media ingestion rate (WW or DW kg/day)

Equation D-1-2 assumes that Ba_A provides a reasonable estimate of the uptake of a compound from incidental ingestion of abiotic media during foraging.

As an example of applying the above equation, *BCF* values for various wildlife measurement receptors listed in Chapter 4 are provided in Table D-2 (water) and Table D-3 (soil and sediment). Measurement-receptor specific ingestion rates used to calculate *BCF*s are presented in Table 5-1. *Ba* values applicable to the mammal and bird measurement receptors for which values were calculated are discussed in Sections D-1.1 and D-1.2, respectively.

BCFs for Dioxins and Furans As discussed in Chapter 2, the *BCF* values for PCDDs and PCDFs are calculated using bioaccumulation equivalency factors (*BEF*s). Consistent with U.S. EPA (1995b), *BEF*s are expressed relative to the *BCF* for 2,3,7,8-TCDD as follows:

$$BCF_j = BCF_{2,3,7,8\text{-}TCDD} \cdot BEF_j \qquad \text{Equation D-1-3}$$

where

BCF_j = Food item-to-animal or media-to-animal *BCF* for *j*th PCDD or PCDF congener for food item-to-animal pathway [(mg COPC/kg FW tissue)/(mg COPC/kg FW plant)]or media-to-animal pathway [(mg COPC/kg FW tissue)/(mg COPC/kg WW media)]

$BCF_{2,3,7,8\text{-}TCDD}$ = Food item-to-animal or media-to-animal *BCF* for 2,3,7,8-TCDD

$BEFj$ = Bioaccumulation equivalency factor for *j*th PCDD or PCDF congener (unitless)

The use of *BEF*s for dioxin and furan congeners is further discussed in Chapter 2.

D-1.1 BIOTRANSFER FACTORS FOR MAMMALS (Ba_{mammal})

As discussed in Section D-1.0, calculation of *BCF* values to be used in pathways for mammals ingesting food items and media requires the determination of COPC-specific biotransfer factors for mammal measurement receptors (Ba_{mammal}). This section discusses selection of the Ba_{mammal} values used to calculate the COPC and measurement receptor specific BCF values presented in Tables D-1 through D-3.

Organics For organics (except PCDDs and PCDFs), the following correlation equation from Travis and Arms (1988) was used to derrive Ba_{mammal} values on a FW basis:

$$\log Ba_{mammal} = -7.6 + \log K_{ow} \qquad \text{Equation D-1-4}$$

where

Ba_{mammal}	=	Biotransfer factor for mammals (day/kg FW tissue)
K_{ow}	=	Octanol-water partition coefficient (unitless)

To calculate the values presented in Tables D-1 through D-3, COPC-specific K_{ow} values were obtained from Appendix A-2.

Biotransfer factors obtained from Travis and Arms (1988) were derived from correlation equations developed from data on experiments conducted with beef cattle ingesting food items and media containing compound classes such as DDT, pesticides, PCDDs, PCDFs, and PCBs. As further literature is developed for other species and compounds, the Travis and Arms (1988) correlation equation should be compared for applicability to species and compound, and best fit correlation for estimation of uptake.

PCDDs and PCDFs Ba_{mammal} values for PCDD and PCDFs were derrived from *Ba* values for cattle as presented in:

- U.S. EPA 1995a. "Further Studies for Modeling the Indirect Exposure Impacts from Combustor Emissions." Memorandum from Matthew Lorber, Exposure Assessment Group, and Glenn Rice, Environmental Criteria and Assessment Office, Washington, D.C. January 20.

U.S. EPA (1995a) determined *Ba* values for cattle from McLachlan, Thoma, Reissinger, and Hutzinger (1990). These empirically determined *Ba* values were recommended by U.S. EPA (1995a) over the Travis and Arms (1988) correlation equation for dioxins and furans.

Inorganics For metals (except cadmium, mercury, selenium, and zinc), *Ba* values on a fresh weight basis were obtained from Baes, Sharp, Sjoreen, and Shor (1984). For cadmium, selenium, and zinc, U.S. EPA (1995a) indicated that *Ba* values were derived by dividing uptake slopes [(g compound/kg DW tissue)/(g compound/kg DW feed)], obtained from U.S. EPA (1992), by a daily consumption rate of 20 kilograms DW per day by cows.

For use in calculating *BCF* values presented in Tables D-1 through D-3 of this appendix, dry weight *Ba* values were converted to fresh weight basis by assuming a tissue moisture content (by mass) of 70 percent for cows. Moisture content information was obtained from the following:

- U.S. EPA. 1997a. *Exposure Factors Handbook*. "Food Ingestion Factors". Volume II. EPA/600/P-95/002Fb. August.

- Pennington, J.A.T. 1994. *Food Value of Portions Commonly Used*. Sixteenth Edition. J.B. Lippincott Company, Philadelphia.

Mercuric Compounds Based on assumptions made regarding speciation and fate and transport of mercury from stack emissions (as discussed in Chapter 2), elemental mercury is assumed not to deposit onto soils, water, or plants. Therefore, it is also not available in food items or media for ingestion and subsequent uptake by measurement receptors. As a result, no *BCF* values for elemental mercury are

presented in Tables D-1 through D-3 of this appendix. If site-specific field data suggest otherwise, *Ba* values for elemental mercury can be derived from uptake slope factors provided in U.S. EPA (1992) and U.S. EPA (1995a), using the same consumption rates as were discussed earlier for the metals like cadmium, selenium, and zinc.

Ba_{mammal} values for mercuric chloride and methyl mercury were derived from data in U.S. EPA (1997b). U.S. EPA (1997b) provides *Ba* values for mercury in cows, but does not specify the form of mercury. To obtain the *Ba* values for mercuric chloride and methyl mercury presented in Tables D-1 through D-3 of this guidance, consistent with U.S. EPA (1997b) total mercury was assumed to be composed of 87 percent divalent mercury (as mercuric chloride) and 13 percent methyl mercury in herbivore animal tissue. Also, assuming that the *Ba* value provided in U.S. EPA (1997b) is for the total mercury in the animal tissue, then biotransfer factors in U.S. EPA (1997b) can be determined for mercuric chloride and methyl mercury, as follows:

- The default *Ba* value of 0.02 day/kg DW for total mercury obtained from U.S. EPA (1997b) was converted to a fresh weight basis assuming a 70 percent moisture content in cow tissue (U.S. EPA 1997a; Pennington 1994). The fresh weight *Ba* value for total mercury was multiplied by 0.13 to obtain a Ba_{mammal} value for methyl mercury, and by 0.87 to obtain a Ba_{mammal} value for mercuric chloride.

D-1.2 BIOTRANSFER FACTORS FOR BIRDS (Ba_{bird})

As discussed in Section D-1.0, calculation of *BCF* values to be used in pathways for birds ingesting food items and media requires the determination of COPC-specific biotransfer factors for bird measurement receptors (Ba_{bird}). This section discusses selection of the Ba_{bird} values used to calculate the COPC and measurement receptor specific *BCF* values presented in Tables D-1 through D-3.

Organics Ba_{bird} values for organic compounds (except PCDDs and PCDFs) were derived from Ba_{mammal} values by assuming that the lipid content (by mass) of birds and mammals is 15 and 19 percent, respectively. Therefore, Ba_{bird} values presented in Tables D-1 through D-3 were determined by multiplying Ba_{mammal} values by the bird and mammal fat content ratio of 0.8 (15/19).

Notable uncertainties associated with this approach include (1) extent to which specific organic compounds bioconcentrate in fatty tissues, and (2) differences in lipid content, metabolism, and feeding characteristics between species.

PCDDs and PCDFs Ba_{bird} values presented in Tables D-1 through D-3 for PCDD and PCDF congeners were derrived from data provided in the following:

- Stephens, R.D., M. Petreas, and G.H. Hayward. 1995. "Biotransfer and Bioaccumulation of Dioxins and Furans from Soil: Chickens as a Model for Foraging Animals." *The Science of the Total Environment.* Volume 175. Pages 253-273.

Stephens, Petreas, and Hayward (1995) conducted experiments to determine the bioavailability and the rate of PCDDs and PCDFs uptake from soil by foraging chickens. Three groups of White Leghorn

chickens were studied—control group, low exposure group, and high exposure group. Eggs, tissues (liver, adipose, and thigh), feed, and feces were analyzed.

Congener specific Ba_{bird} values were derrived from the Stephens, Petreas, and Hayward (1995) study by dividing estimated whole body bioconcentration values for the high exposure group by a daily consumption rate of soil. If congener specific *BCF* values were not reported for the high exposure group, then estimated whole body values were determined using reported data for the low exposure group, if available. A default consumption rate of soil by chicken of 0.02 kg DW/day was determined as follows:

(1) Consumption rate of feed by chicken was obtained from U.S. EPA (1995a), which cites a value of 0.2 kg (DW) feed/day obtained from various literature sources.

(2) The fraction of feed that is soil (0.1) was obtained from Stephens, Petreas, and Hayward (1995).

(3) Feed consumption rate of 0.2 kg/day was multiplied by fraction of feed that is soil (0.1), to obtain the soil consumption rate by chicken of 0.2 x 0.1 = 0.02 kg DW soil/day.

Inorganics For metals (except cadmium, selenium, and zinc), Ba_{bird} values were not available in the literature. For cadmium, selenium, and zinc, U.S. EPA (1995a) cites *Ba* values that were derived by dividing uptake slopes [(g compound/kg dry DW tissue)/(g compound/kg DW feed)], obtained from U.S. EPA (1992), by a daily ingestion rate of 0.2 kilograms DW per day by poultry. To determine *BCF* values presented in Tables D-1 through D-3 in this appendix, reported dry weight *Ba* values were converted to fresh weight basis by assuming a tissue moisture content (by mass) of 75 percent for poultry (U.S. EPA 1997a; Pennington 1994).

Mercuric Compounds Based on assumptions made regarding speciation and fate and transport of mercury from stack emissions (as discussed in Chapter 2), elemental mercury is assumed not to deposit onto soils, water, or plants. Therefore, it is also not available in food items or media for ingestion and subsequent uptake by measurement receptors. As a result, no *BCF* values for elemental mercury are presented in Tables D-1 through D-3 of this appendix. If site-specific field data suggest otherwise, *Ba* values for elemental mercury can be derived from uptake slope factors provided in U.S. EPA (1992) and U.S. EPA (1995a), using the same consumption rates as were discussed earlier for the metals like cadmium, selenium, and zinc.

Ba_{bird} values for mercuric chloride and methyl mercury were derived from data in U.S. EPA (1997b). U.S. EPA (1997b) provides *Ba* values for mercury in poultry, but does not specify the form of mercury. To obtain the *Ba* values for mercuric chloride and methyl mercury presented in Tables D-1 through D-3 of this guidance, consistent with U.S. EPA (1997b) total mercury was assumed to be composed of 87 percent divalent mercury (as mercuric chloride) and 13 percent methyl mercury in herbivore animal tissue. Also, assuming that the *Ba* value provided in U.S. EPA (1997b) is for the total mercury in the animal tissue, then biotransfer factors in U.S. EPA (1997b) can be determined for mercuric chloride and methyl mercury, as follows:

- The default *Ba* value of 0.02 day/kg DW for total mercury obtained from U.S. EPA (1997b) was converted to a fresh weight basis assuming a 75 percent moisture content in poultry tissue (U.S. EPA 1997a; Pennington 1994). The fresh weight *Ba* value for total mercury was multiplied by 0.13 to obtain a Ba_{bird} value for methyl mercury, and by 0.87 to obtain a Ba_{bird} value for mercuric chloride.

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TABLES OF MEASUREMENT RECEPTOR *BCF* VALUES

Screening Level Ecological Risk Assessment Protocol

August 1999

TABLE D-1

BIOCONCENTRATION FACTORS FOR PLANTS TO WILDLIFE MEASUREMENT RECEPTORS

(Page 1 of 3)

Compound	Measurement Receptor													
	American Robin (BCF_{TP-OB})	Canvas Back (BCF_{TP-HB})	Deer Mouse (BCF_{TP-HM})	Least Shrew (BCF_{TP-OM})	Mallard Duck (BCF_{TP-OB})	Marsh Rice Rat (BCF_{TP-OM})	Marsh Wren (BCF_{TP-OB})	Mourning Dove (BCF_{TP-HB})	Muskrat (BCF_{TP-OM})	Northern Bobwhite (BCF_{TP-OB})	Salt-marsh Harvest Mouse (BCF_{TP-HM})	Short-tailed Shrew (BCF_{TP-OM})	Western Meadow Lark (BCF_{TP-OM})	White-footed Mouse (BCF_{TP-OM})
Dioxins and Furans														
2,3,7,8-TCDD	1.53e+02	6.85e+01	3.25e-02	3.37e-02	6.16e+01	2.39e-02	3.19e+02	1.20e+02	1.45e-02	1.20e+02	4.02e-02	3.37e-02	1.45e+02	3.33e-02
1,2,3,7,8-PeCDD	1.41e+02	6.30e+01	2.99e-02	3.10e-02	5.67e+01	2.20e-02	2.93e+02	1.11e+02	1.33e-02	1.11e+02	3.70e-02	3.10e-02	1.33e+02	3.07e-02
1,2,3,4,7,8-HxCDD	4.74e+01	2.12e+01	1.01e-02	1.04e-02	1.91e+01	7.41e-03	9.88e+01	3.72e+01	4.50e-03	3.72e+01	1.25e-02	1.04e-02	4.49e+01	1.03e-02
1,2,3,6,7,8-HxCDD	1.83e+01	8.22e+00	3.91e-03	4.04e-03	7.39e+00	2.87e-03	3.83e+01	1.44e+01	1.74e-03	1.44e+01	4.83e-03	4.04e-03	1.74e+01	4.00e-03
1,2,3,7,8,9-HxCDD	2.14e+01	9.59e+00	4.56e-03	4.71e-03	8.63e+00	3.35e-03	4.46e+01	1.68e+01	2.03e-03	1.68e+01	5.63e-03	4.71e-03	2.03e+01	4.67e-03
1,2,3,4,6,7,8-HpCDD	7.79e+00	3.49e+00	1.66e-03	1.72e-03	3.14e+00	1.22e-03	1.63e+01	6.13e+00	7.40e-04	6.13e+00	2.05e-03	1.72e-03	7.39e+00	1.70e-03
OCDD	1.83e+00	8.22e-01	3.91e-04	4.04e-04	7.39e-01	2.87e-04	3.83e+00	1.44e+00	1.74e-04	1.44e+00	4.83e-04	4.04e-04	1.74e+00	4.00e-04
2,3,7,8-TCDF	1.22e+02	5.48e+01	2.60e-02	2.69e-02	4.93e+01	1.91e-02	2.55e+02	9.61e+01	1.16e-02	9.61e+01	3.22e-02	2.69e-02	1.16e+02	2.67e-02
1,2,3,7,8-PeCDF	3.36e+01	1.51e+01	7.16e-03	7.41e-03	1.36e+01	5.26e-03	7.01e+01	2.64e+01	3.19e-03	2.64e+01	8.85e-03	7.41e-03	3.19e+01	7.34e-03
2,3,4,7,8-PeCDF	2.44e+02	1.10e+02	5.21e-02	5.39e-02	9.86e+01	3.83e-02	5.10e+02	1.92e+02	2.32e-02	1.92e+02	6.44e-02	5.39e-02	2.32e+02	5.34e-02
1,2,3,4,7,8-HxCDF	1.16e+01	5.21e+00	2.47e-03	2.56e-03	4.68e+00	1.82e-03	2.42e+01	9.13e+00	1.10e-03	9.13e+00	3.06e-03	2.56e-03	1.10e+01	2.53e-03
1,2,3,6,7,8-HxCDF	2.90e+01	1.30e+01	6.18e-03	6.40e-03	1.17e+01	4.54e-03	6.06e+01	2.28e+01	2.76e-03	2.28e+01	7.64e-03	6.40e-03	2.75e+01	6.34e-03
2,3,4,6,7,8-HxCDF	1.02e+02	4.59e+01	2.18e-02	2.26e-02	4.13e+01	1.60e-02	2.14e+02	8.05e+01	9.72e-03	8.05e+01	2.70e-02	2.26e-02	9.70e+01	2.23e-02
1,2,3,7,8,9-HxCDF	9.63e+01	4.32e+01	2.05e-02	2.12e-02	3.88e+01	1.51e-02	2.01e+02	7.57e+01	9.14e-03	7.57e+01	2.53e-02	2.12e-02	9.13e+01	2.10e-02
1,2,3,4,6,7,8-HpCDF	1.68e+00	7.54e-01	3.58e-04	3.70e-04	6.78e-01	2.63e-04	3.51e+00	1.32e+00	1.60e-04	1.32e+00	4.43e-04	3.70e-04	1.59e+00	3.67e-04
1,2,3,4,7,8,9-HpCDF	5.96e+01	2.67e+01	1.27e-02	1.31e-02	2.40e+01	9.33e-03	1.24e+02	4.69e+01	5.66e-03	4.69e+01	1.57e-02	1.31e-02	5.65e+01	1.30e-02
OCDF	2.44e+00	1.10e+00	5.21e-04	5.39e-04	9.86e-01	3.83e-04	5.10e+00	1.92e+00	2.32e-04	1.92e+00	6.44e-04	5.39e-04	2.32e+00	5.34e-04
Polynuclear Aromatic Hydrocarbons (PAHs)														
Benzo(a)pyrene	1.19e-02	5.32e-03	2.03e-02	2.10e-02	4.78e-03	1.49e-02	2.47e-02	9.32e-03	9.03e-03	9.32e-03	2.50e-02	2.10e-02	1.12e-02	2.08e-02
Benzo(a)anthracene	4.20e-03	1.88e-03	7.19e-03	7.44e-03	1.69e-03	5.28e-03	8.76e-03	3.30e-03	3.21e-03	3.30e-03	8.89e-03	7.44e-03	3.98e-03	7.37e-03
Benzo(b)fluoranthene	1.40e-02	6.29e-03	2.40e-02	2.48e-02	5.66e-03	1.76e-02	2.93e-02	1.10e-02	1.07e-02	1.10e-02	2.96e-02	2.48e-02	1.33e-02	2.46e-02
Benzo(k)fluoranthene	1.39e-02	6.25e-03	2.39e-02	2.47e-02	5.62e-03	1.75e-02	2.91e-02	1.10e-02	1.06e-02	1.10e-02	2.95e-02	2.47e-02	1.32e-02	2.44e-02
Chrysene	4.84e-03	2.17e-03	8.27e-03	8.56e-03	1.95e-03	6.08e-03	1.01e-02	3.81e-03	3.69e-03	3.81e-03	1.02e-02	8.56e-03	4.59e-03	8.47e-03
Dibenz(a,h)anthracene	3.11e-02	1.39e-02	5.31e-02	5.49e-02	1.25e-02	3.90e-02	6.48e-02	2.44e-02	2.37e-02	2.44e-02	6.57e-02	5.49e-02	2.95e-02	5.44e-02
Indeno(1,2,3-cd)pyrene	7.24e-02	3.25e-02	1.24e-01	1.28e-01	2.92e-02	9.12e-02	1.51e-01	5.69e-02	5.53e-02	5.69e-02	1.53e-01	1.28e-01	6.86e-02	1.27e-01
Polychlorinated Biphenyls (PCBs)														
Aroclor, 1016	2.23e-03	1.00e-03	3.82e-03	3.95e-03	9.01e-04	2.81e-03	4.66e-03	1.76e-03	1.70e-03	1.76e-03	4.72e-03	3.95e-03	2.12e-03	3.91e-03
Aroclor, 1254	1.42e-02	6.35e-03	2.43e-02	2.51e-02	5.71e-03	1.78e-02	2.96e-02	1.11e-02	1.08e-02	1.11e-02	3.00e-02	2.51e-02	1.34e-02	2.49e-02
Nitroaromatics														
1,3-Dinitrobenzene	2.73e-07	1.22e-07	4.67e-07	4.83e-07	1.10e-07	3.43e-07	5.70e-07	2.15e-07	2.08e-07	2.15e-07	5.77e-07	4.83e-07	2.59e-07	4.78e-07
2,4-Dinitrotoluene	8.70e-07	3.90e-07	1.49e-06	1.54e-06	3.51e-07	1.10e-06	1.82e-06	6.84e-07	6.65e-07	6.84e-07	1.85e-06	1.54e-06	8.25e-07	1.53e-06

TABLE D-1

BIOCONCENTRATION FACTORS FOR PLANTS TO WILDLIFE MEASUREMENT RECEPTORS

(Page 2 of 3)

Compound	Measurement Receptor													
	American Robin (BCF_{TP-OB})	Canvas Back (BCF_{TP-HB})	Deer Mouse (BCF_{TP-HM})	Least Shrew (BCF_{TP-OM})	Mallard Duck (BCF_{TP-OB})	Marsh Rice Rat (BCF_{TP-OM})	Marsh Wren (BCF_{TP-OB})	Mourning Dove (BCF_{TP-HB})	Muskrat (BCF_{TP-OM})	Northern Bobwhite (BCF_{TP-OB})	Salt-marsh Harvest Mouse (BCF_{TP-HM})	Short-tailed Shrew (BCF_{TP-OM})	Western Meadow Lark (BCF_{TP-OM})	White-footed Mouse (BCF_{TP-OM})
2,6-Dinitrotoluene	6.79e-07	3.05e-07	1.16e-06	1.20e-06	2.74e-07	8.50e-07	1.42e-06	5.34e-07	5.16e-07	5.34e-07	1.43e-06	1.20e-06	6.44e-07	1.19e-06
Nitrobenzene	5.99e-07	2.69e-07	1.03e-06	1.06e-06	2.42e-07	7.53e-07	1.25e-06	4.71e-07	4.57e-07	4.71e-07	1.27e-06	1.06e-06	5.68e-07	1.05e-06
Pentachloronitrobenzene	3.85e-04	1.72e-04	6.59e-04	6.82e-04	1.55e-04	4.84e-04	8.02e-04	3.02e-04	2.94e-04	3.02e-04	8.15e-04	6.82e-04	3.65e-04	6.76e-04
Phthalate Esters														
Bis(2-ethylhexyl)phthalate	1.41e-03	6.33e-04	2.42e-03	2.50e-03	5.69e-04	1.77e-03	2.95e-03	1.11e-03	1.08e-03	1.11e-03	2.99e-03	2.50e-03	1.34e-03	2.47e-03
Di(n)octyl phthalate	1.88e+01	8.44e+00	3.22e+01	3.33e+01	7.59e+00	2.36e+01	3.93e+01	1.48e+01	1.43e+01	1.48e+01	3.98e+01	3.33e+01	1.78e+01	3.30e+01
Volatile Organic Compounds														
Acetone	5.28e-09	2.37e-09	9.05e-09	9.36e-09	2.13e-09	6.65e-09	1.10e-08	4.15e-09	4.03e-09	4.15e-09	1.12e-08	9.36e-09	5.01e-09	9.27e-09
Acrylonitrile	1.57e-08	7.03e-09	2.68e-08	2.77e-08	6.32e-09	1.97e-08	3.27e-08	1.23e-08	1.19e-08	1.23e-08	3.31e-08	2.77e-08	1.49e-08	2.75e-08
Chloroform	7.82e-07	3.50e-07	1.34e-06	1.39e-06	3.15e-07	9.87e-07	1.63e-06	6.14e-07	5.98e-07	6.14e-07	1.66e-06	1.39e-06	7.41e-07	1.38e-06
Crotonaldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
1,4-Dioxane	4.75e-09	2.13e-09	8.15e-09	8.43e-09	1.92e-09	5.99e-09	9.91e-09	3.74e-09	3.63e-09	3.74e-09	1.01e-08	8.43e-09	4.50e-09	8.35e-09
Formaldehyde	1.94e-08	8.68e-09	3.31e-08	3.43e-08	7.81e-09	2.44e-08	4.04e-08	1.52e-08	1.48e-08	1.52e-08	4.10e-08	3.43e-08	1.84e-08	3.40e-08
Vinyl chloride	1.23e-07	5.53e-08	2.11e-07	2.18e-07	4.98e-08	1.55e-07	2.58e-07	9.71e-08	9.40e-08	9.71e-08	2.61e-07	2.18e-07	1.17e-07	2.16e-07
Other Chlorinated Organics														
Hexachlorobenzene	2.80e-03	1.26e-03	4.79e-03	4.95e-03	1.13e-03	3.52e-03	5.85e-03	2.20e-03	2.13e-03	2.20e-03	5.92e-03	4.95e-03	2.66e-03	4.91e-03
Hexachlorobutadiene	4.75e-04	2.13e-04	8.09e-04	8.37e-04	1.92e-04	5.95e-04	9.91e-04	3.74e-04	3.61e-04	3.74e-04	1.00e-03	8.37e-04	4.50e-04	8.29e-04
Hexachlorocyclopentadiene	7.11e-04	3.19e-04	1.22e-03	1.26e-03	2.87e-04	8.94e-04	1.48e-03	5.59e-04	5.42e-04	5.59e-04	1.50e-03	1.26e-03	6.74e-04	1.25e-03
Pentachlorobenzene	1.08e-03	4.84e-04	1.84e-03	1.90e-03	4.35e-04	1.35e-03	2.25e-03	8.48e-04	8.20e-04	8.48e-04	2.27e-03	1.90e-03	1.02e-03	1.89e-03
Pentachlorophenol	1.06e-03	4.76e-04	1.81e-03	1.87e-03	4.28e-04	1.33e-03	2.21e-03	8.34e-04	8.07e-04	8.34e-04	2.24e-03	1.87e-03	1.01e-03	1.85e-03
Pesticides														
4,4-DDE	1.59e-02	7.13e-03	2.72e-02	2.81e-02	6.41e-03	2.00e-02	3.32e-02	1.25e-02	1.21e-02	1.25e-02	3.36e-02	2.81e-02	1.51e-02	2.78e-02
Heptachlor	9.10e-04	4.08e-04	1.56e-03	1.61e-03	3.67e-04	1.15e-03	1.90e-03	7.16e-04	6.95e-04	7.16e-04	1.93e-03	1.61e-03	8.63e-04	1.60e-03
Hexachlorophene	3.06e-01	1.37e-01	5.22e-01	5.40e-01	1.23e-01	3.84e-01	6.37e-01	2.40e-01	2.33e-01	2.40e-01	6.45e-01	5.40e-01	2.90e-01	5.35e-01
Inorganics														
Aluminum	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Antimony	NA	NA	5.99e-04	6.20e-04	NA	4.40e-04	NA	NA	2.67e-04	NA	7.41e-04	6.20e-04	NA	6.14e-04
Arsenic	NA	NA	1.20e-03	1.24e-03	NA	8.81e-04	NA	NA	5.34e-04	NA	1.48e-03	1.24e-03	NA	1.23e-03
Barium	NA	NA	8.99e-05	9.30e-05	NA	6.61e-05	NA	NA	4.01e-05	NA	1.11e-04	9.30e-05	NA	9.21e-05
Beryllium	NA	NA	5.99e-04	6.20e-04	NA	4.40e-04	NA	NA	2.67e-04	NA	7.41e-04	6.20e-04	NA	6.14e-04
Cadmium	4.71e-02	2.11e-02	7.19e-05	7.44e-05	1.90e-02	5.28e-05	9.82e-02	3.70e-02	3.21e-05	3.70e-02	8.89e-05	7.44e-05	4.46e-02	7.37e-05
Chromium (hexavalent)	NA	NA	3.30e-03	3.41e-03	NA	2.42e-03	NA	NA	1.47e-03	NA	4.08e-03	3.41e-03	NA	3.38e-03

TABLE D-1

BIOCONCENTRATION FACTORS FOR PLANTS TO WILDLIFE MEASUREMENT RECEPTORS

(Page 3 of 3)

Compound	Measurement Receptor													
	American Robin (BCF_{TP-OB})	Canvas Back (BCF_{TP-HB})	Deer Mouse (BCF_{TP-HM})	Least Shrew (BCF_{TP-OM})	Mallard Duck (BCF_{TP-OB})	Marsh Rice Rat (BCF_{TP-OM})	Marsh Wren (BCF_{TP-OB})	Mourning Dove (BCF_{TP-HB})	Muskrat (BCF_{TP-OM})	Northern Bobwhite (BCF_{TP-OB})	Salt-marsh Harvest Mouse (BCF_{TP-HM})	Short-tailed Shrew (BCF_{TP-OM})	Western Meadow Lark (BCF_{TP-OM})	White-footed Mouse (BCF_{TP-OM})
Copper	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Total Cyanide	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lead	NA	NA	1.80e-04	1.86e-04	NA	1.32e-04	NA	NA	8.02e-05	NA	2.22e-04	1.86e-04	NA	1.84e-04
Mercuric chloride	1.06e-02	4.76e-03	3.13e-03	3.24e-03	4.28e-03	2.30e-03	2.21e-02	8.34e-03	1.39e-03	8.34e-03	3.87e-03	3.24e-03	1.01e-02	3.21e-03
Methylmercury	1.59e-03	7.13e-04	4.68e-04	4.84e-04	6.41e-04	3.44e-04	3.32e-03	1.25e-03	2.08e-04	1.25e-03	5.78e-04	4.84e-04	1.51e-03	4.79e-04
Nickel	NA	NA	3.60e-03	3.72e-03	NA	2.64e-03	NA	NA	1.60e-03	NA	4.45e-03	3.72e-03	NA	3.68e-03
Selenium	5.02e-01	2.25e-01	1.36e-03	1.41e-03	2.02e-01	1.00e-03	1.05e+00	3.95e-01	6.07e-04	3.95e-01	1.68e-03	1.41e-03	4.76e-01	1.39e-03
Silver	NA	NA	1.80e-03	1.86e-03	NA	1.32e-03	NA	NA	8.02e-04	NA	2.22e-03	1.86e-03	NA	1.84e-03
Thallium	NA	NA	2.40e-02	2.48e-02	NA	1.76e-02	NA	NA	1.07e-02	NA	2.96e-02	2.48e-02	NA	2.46e-02
Zinc	3.89e-03	1.74e-03	5.39e-05	5.58e-05	1.57e-03	3.96e-05	8.11e-03	3.05e-03	2.40e-05	3.05e-03	6.67e-05	5.58e-05	3.68e-03	5.53e-05

Notes:

NA - Indicates insufficient data to determine value

HB - Herbivorous bird
HM - Herbivorous mammal
OB - Omnivorous bird
OM - Omnivorous mammal
TP - Terrestrial plant

– Values provided were determined as specified in the text of Appendix D. *BCF* values for omnivores were determined based on an equal diet. *BCF* values for dioxin and furan congeners determined using BEF values specified in Chapter 2.

Table D-2

Bioconcentration Factors for Water to Wildlife Measurement Receptors

(Page 1 of 6)

Compound	Measurement Receptors										
	American Kestrel (BCF_{W-CB})	American Robin (BCF_{W-OB})	Canvas Back (BCF_{W-HB})	Deer Mouse (BCF_{W-HM})	Least Shrew (BCF_{W-OM})	Long-tailed Weasel (BCF_{W-OM})	Mallard Duck (BCF_{W-OB})	Marsh Rice Rat (BCF_{W-OM})	Marsh Wren (BCF_{W-OB})	Mink (BCF_{W-CM})	Mourning Dove (BCF_{W-OM})
Dioxins and Furans											
2,3,7,8-TCDD	4.30e+01	4.71e+01	2.21e+01	8.19e-03	9.34e-03	6.88e-03	2.00e+01	1.03e-02	9.46e+01	5.39e-03	3.75e+01
1,2,3,7,8-PeCDD	3.96e+01	4.34e+01	2.04e+01	7.54e-03	8.59e-03	6.33e-03	1.84e+01	9.44e-03	8.70e+01	4.96e-03	3.45e+01
1,2,3,4,7,8-HxCDD	1.33e+01	1.46e+01	6.86e+00	2.54e-03	2.89e-03	2.13e-03	6.21e+00	3.18e-03	2.93e+01	1.67e-03	1.16e+01
1,2,3,6,7,8-HxCDD	5.16e+00	5.66e+00	2.65e+00	9.83e-04	1.12e-03	8.25e-04	2.40e+00	1.23e-03	1.14e+01	6.47e-04	4.50e-01
1,2,3,7,8,9-HxCDD	6.02e+00	6.60e+00	3.10e+00	1.15e-03	1.31e-03	9.63e-04	2.80e+00	1.44e-03	1.32e+01	7.55e-04	5.25e+00
1,2,3,4,6,7,8-HpCDD	2.19e+00	2.40e+00	1.13e+00	4.18e-04	4.76e-04	3.51e-04	1.02e+00	5.23e-04	4.82e+00	2.75e-04	1.91e+00
OCDD	5.16e-01	5.66e-01	2.65e-01	9.83e-05	1.12e-04	8.25e-05	2.40e-01	1.23e-04	1.14e+00	6.47e-05	4.50e-01
2,3,7,8-TCDF	3.44e+01	3.77e+01	1.77e+01	6.55e-03	7.47e-03	5.50e-03	1.60e+01	8.21e-03	7.57e+01	4.31e-03	3.00e+01
1,2,3,7,8-PeCDF	9.46e+00	1.04e+01	4.87e+00	1.80e-03	2.05e-03	1.51e-03	4.40e+00	2.26e-03	2.08e+01	1.19e-03	8.25e+00
2,3,4,7,8-PeCDF	6.88e+01	7.54e+01	3.54e+01	1.31e-02	1.49e-02	1.10e-02	3.20e+01	1.64e-02	1.51e+02	8.62e-03	6.00e+01
1,2,3,4,7,8-HxCDF	3.27e+00	3.58e+00	1.68e+00	6.23e-04	7.10e-04	5.23e-04	1.52e+00	7.80e-04	7.19e+00	4.10e-04	2.85e+00
1,2,3,6,7,8-HxCDF	8.17e+00	8.95e+00	4.20e+00	1.56e-03	1.77e-03	1.31e-03	3.80e+00	1.95e-03	1.80e+01	1.02e-03	7.12e+00
2,3,4,6,7,8-HxCDF	2.88e+01	3.16e+01	1.48e+01	5.49e-03	6.26e-03	4.61e-03	1.34e+01	6.88e-03	6.34e+01	3.61e-03	2.51e+01
1,2,3,7,8,9-HxCDF	2.71e+01	2.97e+01	1.39e+01	5.16e-03	5.88e-03	4.33e-03	1.26e+01	6.47e-03	5.96e+01	3.40e-03	2.36e+01
1,2,3,4,6,7,8-HpCDF	4.73e-01	5.18e-01	2.43e-01	9.01e-05	1.03e-04	7.57e-05	2.20e-01	1.13e-04	1.04e+00	5.93e-05	4.12e-01
1,2,3,4,7,8,9-HpCDF	1.68e+01	1.84e+01	8.63e+00	3.20e-03	3.64e-03	2.68e-03	7.81e+00	4.00e-03	3.69e+01	2.10e-03	1.46e+01
OCDF	6.88e-01	7.54e-01	3.54e-01	1.31e-04	1.49e-04	1.10e-04	3.20e-01	1.64e-04	1.51e+00	8.62e-05	6.00e-01
Polynuclear Aromatic Hydrocarbons (PAHs)											
Benzo(a)pyrene	3.34e-03	3.67e-03	1.72e-03	5.10e-03	5.81e-03	4.28e-03	1.55e-03	3.75e-03	7.35e-03	3.36e-03	2.92e-03
Benzo(a)anthracene	1.18e-03	1.30e-03	6.08e-04	1.81e-03	2.06e-03	1.52e-03	5.50e-04	1.33e-03	2.60e-03	1.19e-03	1.03e-03
Benzo(b)fluoranthene	3.95e-03	4.34e-03	2.03e-03	6.03e-03	6.88e-03	5.07e-03	1.84e-03	4.44e-03	8.70e-03	3.97e-03	3.46e-03
Benzo(k)fluoranthene	3.92e-03	4.31e-03	2.02e-03	6.00e-03	6.84e-03	5.04e-03	1.83e-03	4.41e-03	8.64e-03	3.95e-03	3.43e-03
Chrysene	1.36e-03	1.50e-03	7.01e-04	2.08e-03	2.37e-03	1.75e-03	6.34e-04	1.53e-03	3.00e-03	1.37e-03	1.19e-03
Dibenz(a,h)anthracene	8.74e-03	9.61e-03	4.50e-03	1.34e-02	1.52e-02	1.12e-02	4.07e-03	9.84e-03	1.93e-02	8.79e-03	7.66e-03
Indeno(1,2,3-cd)pyrene	2.04e-02	2.24e-02	1.05e-02	3.12e-02	3.56e-02	2.62e-02	9.48e-03	2.29e-02	4.49e-02	2.05e-02	1.78e-02
Polychlorinated Biphenyls (PCBs)											
Aroclor 1016	6.28e-04	6.91e-04	3.24e-04	9.61e-04	1.10e-03	8.07e-04	2.93e-04	7.07e-04	1.38e-03	6.32e-04	5.50e-04
Aroclor 1254	3.98e-03	4.38e-03	2.05e-03	6.11e-03	6.96e-03	5.13e-03	1.86e-03	4.48e-03	8.78e-03	4.02e-03	3.49e-03
Nitroaromatics											
1,3-Dinitrobenzene	7.68e-08	8.45e-08	3.96e-08	1.18e-07	1.34e-07	9.87e-08	3.58e-08	8.65e-08	1.69e-07	7.73e-08	6.73e-08
2,4-Dinitrotoluene	2.45e-07	2.69e-07	1.26e-07	3.76e-07	4.28e-07	3.15e-07	1.14e-07	2.76e-07	5.39e-07	2.47e-07	2.14e-07

Table D-2

Bioconcentration Factors for Water to Wildlife Measurement Receptors

(Page 2 of 6)

Compound	Measurement Receptors										
	American Kestrel (BCF_{W-CB})	American Robin (BCF_{W-OB})	Canvas Back (BCF_{W-HB})	Deer Mouse (BCF_{W-HM})	Least Shrew (BCF_{W-OM})	Long-tailed Weasel (BCF_{W-OM})	Mallard Duck (BCF_{W-OB})	Marsh Rice Rat (BCF_{W-OM})	Marsh Wren (BCF_{W-OB})	Mink (BCF_{W-CM})	Mourning Dove (BCF_{W-OM})
2,6-Dinitrotoluene	1.91e-07	2.10e-07	9.84e-08	2.91e-07	3.32e-07	2.44e-07	8.90e-08	2.15e-07	4.21e-07	1.92e-07	1.67e-07
Nitrobenzene	1.69e-07	1.85e-07	8.68e-08	2.58e-07	2.94e-07	2.17e-07	7.86e-08	1.90e-07	3.72e-07	1.70e-07	1.48e-07
Pentachloronitrobenzene	1.08e-04	1.19e-04	5.57e-05	1.66e-04	1.89e-04	1.39e-04	5.04e-05	1.22e-04	2.38e-04	1.09e-04	9.47e-05
Phthalate Esters											
Bis(2-ethylhexyl)phthalate	3.97e-04	4.37e-04	2.05e-04	6.08e-04	6.93e-04	5.11e-04	1.85e-04	4.47e-04	8.75e-04	4.00e-04	3.48e-04
Di(n)octyl phthalate	5.30e+00	5.82e+00	2.73e+00	8.10e+00	9.23e+00	6.80e+00	2.47e+00	5.96e+00	1.17e+01	5.33e+00	4.64e+00
Volatile Organic Compounds											
Acetone	1.49e-09	1.63e-09	7.65e-10	2.28e-09	2.60e-09	1.91e-09	6.92e-10	1.67e-09	3.28e-09	1.50e-09	1.30e-09
Acrylonitrile	4.41e-09	4.84e-09	2.27e-09	6.74e-09	7.69e-09	5.66e-09	2.05e-09	1.27e-09	9.71e-09	4.44e-09	3.85e-09
Chloroform	2.20e-07	2.42e-07	1.13e-07	3.38e-07	3.85e-07	2.84e-07	1.02e-07	2.47e-07	4.84e-07	2.22e-07	1.93e-07
Crotonaldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
1,4-Dioxane	1.34e-09	1.47e-09	6.88e-10	2.05e-09	2.34e-09	1.72e-09	6.23e-10	1.50e-09	2.95e-09	1.35e-09	1.17e-09
Formaldehyde	5.45e-09	5.99e-09	2.80e-09	8.34e-09	9.51e-09	7.01e-09	2.54e-09	6.13e-09	1.20e-08	5.49e-09	4.77e-09
Vinyl chloride	3.47e-08	3.82e-08	1.79e-08	5.31e-08	6.05e-08	4.46e-08	1.62e-08	3.91e-08	7.65e-08	3.49e-08	3.04e-08
Other Chlorinated Organics											
Hexachlorobenzene	7.88e-04	8.67e-04	4.06e-04	1.21e-03	1.37e-03	1.01e-03	3.67e-04	8.87e-04	1.74e-03	7.93e-04	6.90e-04
Hexachlorobutadiene	1.34e-04	1.47e-04	6.88e-05	2.04e-04	2.32e-04	1.71e-04	6.23e-05	1.51e-04	2.94e-04	1.34e-04	1.17e-04
Hexachlorocyclopentadiene	2.00e-04	2.20e-04	1.03e-04	3.06e-04	3.49e-04	2.57e-04	9.31e-05	2.25e-04	4.40e-04	2.02e-04	1.75e-04
Pentachlorobenzene	3.04e-04	3.34e-04	1.56e-04	4.63e-04	5.28e-04	3.89e-04	1.41e-04	3.42e-04	6.69e-04	3.05e-04	2.66e-04
Pentachlorophenol	2.99e-04	3.28e-04	1.54e-04	4.56e-04	5.19e-04	3.83e-04	1.39e-04	3.36e-04	6.58e-04	3.00e-04	2.61e-04
Pesticides											
4,4-DDE	4.47e-03	4.92e-03	2.30e-03	6.83e-03	7.79e-03	5.74e-03	2.08e-03	5.03e-03	9.85e-03	4.50e-03	3.92e-03
Heptachlor	2.56e-04	2.82e-04	1.32e-04	3.92e-04	4.47e-04	3.29e-04	1.19e-04	2.88e-04	5.64e-04	2.58e-04	2.24e-04
Hexachlorophene	8.59e-02	9.45e-02	4.42e-02	1.31e-01	1.50e-01	1.10e-01	4.00e-02	9.67e-02	1.89e-01	8.65e-02	7.53e-02
Inorganics											
Aluminum	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Antimony	NA	NA	NA	1.51e-04	1.72e-04	1.27e-04	NA	NA	NA	9.93e-05	NA
Arsenic	NA	NA	NA	3.02e-04	3.44e-04	2.53e-04	NA	NA	NA	1.99e-04	NA
Barium	NA	NA	NA	2.26e-05	2.58e-05	1.90e-05	NA	NA	NA	1.49e-05	NA
Beryllium	NA	NA	NA	1.51e-04	1.72e-04	1.27e-04	NA	NA	NA	9.93e-05	NA
Cadmium	1.32e-02	1.46e-02	6.82e-03	1.81e-05	2.06e-05	1.52e-05	6.17e-03	1.49e-02	2.92e-02	1.19e-05	1.16e-02
Chromium (hexavalent)	NA	NA	NA	8.30e-04	9.46e-04	6.97e-04	NA	NA	NA	5.46e-04	NA

Table D-2

Bioconcentration Factors for Water to Wildlife Measurement Receptors

(Page 3 of 6)

Compound	Measurement Receptors										
	American Kestrel (BCF_{W-CB})	American Robin (BCF_{W-OB})	Canvas Back (BCF_{W-HB})	Deer Mouse (BCF_{W-HM})	Least Shrew (BCF_{W-OM})	Long-tailed Weasel (BCF_{W-OM})	Mallard Duck (BCF_{W-OB})	Marsh Rice Rat (BCF_{W-OM})	Marsh Wren (BCF_{W-OB})	Mink (BCF_{W-CM})	Mourning Dove (BCF_{W-OM})
Copper	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Total Cyanide	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lead	NA	NA	NA	4.53e-05	5.16e-05	3.80e-05	NA	NA	NA	2.98e-05	NA
Mercuric Chloride	2.99e-03	3.27e-03	1.54e-03	7.88e-04	8.98e-04	6.63e-04	1.39e-03	2.99e-03	6.57e-03	5.18e-04	2.61e-03
Methylmercury	4.48e-04	4.90e-04	2.30e-04	1.18e-04	1.34e-04	9.91e-05	2.08e-04	5.05e-04	9.85e-04	7.74e-05	3.90e-04
Nickel	NA	NA	NA	9.05e-04	1.03e-03	7.60e-04	NA	NA	NA	5.96e-04	NA
Selenium	1.41e-01	1.55e-01	7.27e-02	3.42e-04	3.90e-04	2.88e-04	6.58e-02	1.59e-01	3.11e-01	2.25e-04	1.24e-01
Silver	NA	NA	NA	4.53e-04	5.16e-04	3.80e-04	NA	NA	NA	2.98e-04	NA
Thallium	NA	NA	NA	6.03e-03	6.88e-03	5.07e-03	NA	NA	NA	3.97e-03	NA
Zinc	1.09e-03	1.20e-03	5.63e-04	1.36e-05	1.55e-05	1.14e-05	5.09e-04	1.23e-03	2.41e-03	8.93e-06	9.57e-04

Notes:

NA - Indicates insufficient data to determine value

HB - Herbivorous bird
HM - Herbivorous mammal
OB - Omnivorous bird
OM - Omnivorous mammal
TP - Terrestrial plant

– Values provided were determined as specified in the text of Appendix D. *BCF* values for omnivores were determined based on an equal diet. *BCF* values for dioxin and furan congeners determined using BEF values specified in Chapter 2.

Table D-2

Bioconcentration Factors for Water to Wildlife Measurement Receptors

(Page 4 of 6)

Compound	Measurement Receptors										
	Muskrat (BCF_{W-OM})	Northern Bobwhite (BCF_{W-OB})	Northern Harrier (BCF_{W-CM})	Red Fox (BCF_{W-CM})	Red-tailed Hawk (BCF_{W-HM})	Salt-marsh Harvest Mouse (BCF_{W-HM})	Short-tailed Shrew (BCF_{W-OM})	Spotted Sandpiper (BCF_{W-CSB})	Swift Fox (BCF_{W-OM})	Western Meadow Lark (BCF_{W-OM})	White-footed Mouse (BCF_{W-OM})
Dioxins and Furans											
2,3,7,8-TCDD	5.33e-03	3.75e+01	2.06e+01	4.69e-03	2.06e+01	8.60e-03	8.18e-03	5.99e+01	5.07e-03	4.51e+01	8.24e-03
1,2,3,7,8-PeCDD	4.90e-03	3.45e+01	1.90e+01	4.31e-03	1.90e+01	7.91e-03	7.53e-03	5.51e+01	4.66e-03	4.15e+01	7.58e-03
1,2,3,4,7,8-HxCDD	1.65e-03	1.16e+01	6.39e+00	1.45e-03	6.39e+00	2.67e-03	2.54e-03	1.86e+01	1.57e-03	1.40e+01	2.55e-03
1,2,3,6,7,8-HxCDD	6.40e-05	4.50e+00	2.47e+00	5.62e-04	2.47e+00	1.03e-03	9.82e-04	7.18e+00	6.08e-04	5.41e+00	9.89e-04
1,2,3,7,8,9-HxCDD	7.46e-04	5.25e+00	2.88e+00	6.56e-04	2.88e+00	1.20e-03	1.15e-03	8.38e+00	7.10e-04	6.31e+00	1.15e-03
1,2,3,4,6,7,8-HpCDD	2.72e-04	1.91e+00	1.05e+00	2.39e-04	1.05e+00	4.39e-04	4.17e-04	3.05e+00	2.59e-04	2.30e+00	4.20e-04
OCDD	6.40e-05	4.50e-01	2.47e-01	5.62e-05	2.47e-01	1.03e-04	9.82e-05	7.18e-01	6.08e-05	5.41e-01	9.89e-05
2,3,7,8-TCDF	4.26e-03	3.00e+01	1.65e+01	3.75e-03	1.65e+01	6.88e-03	6.55e-03	4.79e+01	4.06e-03	3.61e+01	6.59e-03
1,2,3,7,8-PeCDF	1.17e-03	8.25e+00	4.53e+00	1.03e-03	4.53e+00	1.89e-03	1.80e-03	1.32e+01	1.12e-03	9.91e+00	1.81e-03
2,3,4,7,8-PeCDF	8.53e-03	6.00e+01	3.30e+01	7.50e-03	3.30e+01	1.38e-02	1.31e-02	9.58e+01	8.11e-03	7.21e+01	1.32e-02
1,2,3,4,7,8-HxCDF	4.05e-04	2.85e+00	1.57e+00	3.56e-04	1.57e+00	6.54e-04	6.22e-04	4.55e+00	3.85e-04	3.42e+00	6.26e-04
1,2,3,6,7,8-HxCDF	1.01e-03	7.12e+00	3.92e+00	8.91e-04	3.92e+00	1.63e-03	1.55e-03	1.14e+01	9.63e-04	8.56e+00	1.57e-03
2,3,4,6,7,8-HxCDF	3.57e-03	2.51e+01	1.38e+01	3.14e-03	1.38e+01	5.76e-03	5.48e-03	4.01e+01	3.40e-03	3.02e+01	5.52e-03
1,2,3,7,8,9-HxCDF	3.36e-03	2.36e+01	1.30e+01	2.95e-03	1.30e+01	5.42e-03	5.15e-03	3.77e+01	3.19e-03	2.84e+01	5.19e-03
1,2,3,4,6,7,8-HpCDF	5.86e-05	4.12e-01	2.27e-01	5.16e-05	2.27e-01	9.46e-05	9.00e-05	6.58e-01	5.58e-05	4.96e-01	9.06e-05
1,2,3,4,7,8,9-HpCDF	2.08e-03	1.46e+01	8.04e+00	1.83e-03	8.04e+00	0.00e+00	3.19e-03	2.33e+01	1.98e-03	1.76e+01	3.21e-03
OCDF	8.53e-05	6.00e-01	3.30e-01	7.50e-05	3.30e-01	1.38e-04	1.31e-04	9.58e-01	8.11e-05	7.21e-01	1.32e-04
Polynuclear aromatic hydrocarbons (PAHs)											
Benzo(a)pyrene	3.32e-03	2.92e-03	1.60e-03	2.92e-03	1.60e-03	5.35e-03	5.09e-03	4.64e-03	3.16e-03	3.49e-03	5.13e-03
Benzo(a)anthracene	1.18e-03	1.03e-03	5.66e-04	1.04e-03	5.66e-04	1.90e-03	1.81e-03	1.64e-03	1.12e-03	1.24e-03	1.82e-03
Benzo(b)fluoranthene	3.93e-03	3.46e-03	1.89e-03	3.45e-03	1.89e-03	6.34e-03	6.03e-03	5.49e-03	3.73e-03	4.13e-03	6.07e-03
Benzo(k)fluoranthene	3.91e-03	3.43e-03	1.88e-03	3.44e-03	1.88e-03	6.30e-03	6.00e-03	5.46e-03	3.72e-03	4.10e-03	6.04e-03
Chrysene	1.35e-03	1.19e-03	6.53e-04	1.19e-03	6.53e-04	2.19e-03	2.08e-03	1.89e-03	1.29e-03	1.42e-03	2.09e-03
Dibenz(a,h)anthracene	8.70e-03	7.66e-03	4.19e-03	7.65e-03	4.19e-03	1.40e-02	1.33e-02	1.22e-02	8.27e-03	9.14e-03	1.34e-02
Indeno(1,2,3-cd)pyrene	2.03e-02	1.78e-02	9.76e-03	1.79e-02	9.76e-03	3.28e-02	3.12e-02	2.83e-02	1.93e-02	2.13e-02	3.14e-02
Polychlorinated biphenyls (PCBs)											
Aroclor 1016	6.25e-04	5.50e-04	3.01e-04	5.50e-04	3.01e-04	1.01e-03	9.60e-04	8.74e-04	5.95e-04	6.57e-04	9.66e-04
Aroclor 1254	3.98e-03	3.49e-03	1.91e-03	3.50e-03	1.91e-03	6.41e-03	6.10e-03	5.54e-03	3.78e-03	4.16e-03	6.14e-03
Nitroaromatics											
1,3-Dinitrobenzene	7.65e-08	6.73e-08	3.68e-08	6.72e-08	3.68e-08	1.23e-07	1.17e-07	1.07e-07	7.27e-08	8.03e-08	1.18e-07
2,4-Dinitrotoluene	2.44e-07	2.14e-07	1.17e-07	2.15e-07	1.17e-07	3.94e-07	3.75e-07	3.41e-07	2.32e-07	2.56e-07	3.78e-07

Table D-2

Bioconcentration Factors for Water to Wildlife Measurement Receptors

(Page 5 of 6)

Compound	Measurement Receptors										
	Muskrat (BCF_{W-OM})	Northern Bobwhite (BCF_{W-OB})	Northern Harrier (BCF_{W-CM})	Red Fox (BCF_{W-CM})	Red-tailed Hawk (BCF_{W-HM})	Salt-marsh Harvest Mouse (BCF_{W-HM})	Short-tailed Shrew (BCF_{W-OM})	Spotted Sandpiper (BCF_{W-CSB})	Swift Fox (BCF_{W-OM})	Western Meadow Lark (BCF_{W-OM})	White-footed Mouse (BCF_{W-OM})
2,6-Dinitrotoluene	1.89e-07	1.67e-07	9.16e-08	1.67e-07	9.16e-08	3.06e-07	2.91e-07	2.66e-07	1.80e-07	2.00e-07	2.93e-07
Nitrobenzene	1.68e-07	1.48e-07	8.08e-08	1.48e-07	8.08e-08	2.71e-07	2.58e-07	2.35e-07	1.60e-07	1.76e-07	2.59e-07
Pentachloronitrobenzene	1.08e-04	9.47e-05	5.18e-05	9.49e-05	5.18e-05	1.74e-04	1.66e-04	1.50e-04	1.03e-04	1.13e-04	1.67e-04
Phthalate Esters											
Bis(2-ethylhexyl)phthalate	3.96e-04	3.48e-04	1.90e-04	3.48e-04	1.90e-04	6.38e-04	6.07e-04	5.52e-04	3.76e-04	4.15e-04	6.11e-04
Di(n)octyl phthalate	5.27e+00	4.64e+00	2.54e+00	4.64e+00	2.54e+00	8.51e+00	8.09e+00	7.37e+00	5.01e+00	5.54e+00	8.15e+00
Volatile Organic Compounds											
Acetone	1.48e-09	1.30e-09	7.12e-10	1.30e-09	7.12e-10	2.39e-09	2.28e-09	2.07e-09	1.41e-09	1.55e-09	2.29e-09
Acrylonitrile	4.39e-09	3.85e-09	2.11e-09	3.86e-09	2.11e-09	7.08e-09	6.73e-09	6.14e-09	4.17e-09	4.62e-09	6.78e-09
Chloroform	2.20e-07	1.93e-07	1.05e-07	1.93e-07	1.05e-07	3.55e-07	3.38e-07	3.06e-07	2.09e-07	2.30e-07	3.40e-07
Crotonaldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
1,4-Dioxane	1.33e-09	1.17e-09	6.41e-10	1.17e-09	6.41e-10	2.15e-09	2.05e-09	1.86e-09	1.27e-09	1.40e-09	2.06e-09
Formaldehyde	5.43e-09	4.77e-09	2.61e-09	4.77e-09	2.61e-09	8.76e-09	8.33e-09	7.58e-09	5.16e-09	5.69e-09	8.39e-09
Vinyl chloride	3.45e-08	3.04e-08	1.66e-08	3.04e-08	1.66e-08	5.58e-08	5.30e-08	4.83e-08	3.29e-08	3.63e-08	5.34e-08
Other Chlorinated Organics											
Hexachlorobenzene	7.84e-04	6.90e-04	3.78e-04	6.90e-04	3.78e-04	1.27e-03	1.20e-03	1.10e-03	7.46e-04	8.24e-04	1.21e-03
Hexachlorobutadiene	1.33e-04	1.17e-04	6.41e-05	1.17e-04	6.41e-05	2.13e-04	2.04e-04	1.86e-04	1.26e-04	1.40e-04	2.05e-04
Hexachlorocyclopentadiene	1.99e-04	1.75e-04	9.58e-05	1.75e-04	9.58e-05	3.22e-04	3.06e-04	2.78e-04	1.90e-04	2.09e-04	3.08e-04
Pentachlorobenzene	3.01e-04	2.66e-04	1.45e-04	2.65e-04	1.45e-04	4.86e-04	4.63e-04	4.22e-04	2.87e-04	3.17e-04	4.66e-04
Pentachlorophenol	2.96e-04	2.61e-04	1.43e-04	2.61e-04	1.43e-04	4.78e-04	4.55e-04	4.15e-04	2.82e-04	3.12e-04	4.58e-04
Pesticides											
4,4-DDE	4.45e-03	3.92e-03	2.14e-03	3.91e-03	2.14e-03	7.18e-03	6.83e-03	6.22e-03	4.23e-03	4.67e-03	6.87e-03
Heptachlor	2.55e-04	2.24e-04	1.23e-04	2.24e-04	1.23e-04	4.12e-04	3.92e-04	3.56e-04	2.43e-04	2.68e-04	3.94e-04
Hexachlorophene	8.55e-02	7.53e-02	4.12e-02	7.52e-02	4.12e-02	1.38e-01	1.31e-01	1.20e-01	8.13e-02	8.98e-02	1.32e-01
Inorganics											
Aluminum	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Antimony	9.82e-05	NA	NA	8.63e-05	NA	1.58e-04	1.51e-04	NA	9.33e-05	NA	1.52e-04
Arsenic	1.96e-04	NA	NA	1.73e-04	NA	3.17e-04	3.01e-04	NA	1.87e-04	NA	3.03e-04
Barium	1.47e-05	NA	NA	1.29e-05	NA	2.38e-05	2.26e-05	NA	1.40e-05	NA	2.28e-05
Beryllium	9.82e-05	NA	NA	8.63e-05	NA	1.58e-04	1.51e-04	NA	9.33e-05	NA	1.52e-04
Cadmium	1.18e-05	1.16e-02	6.35e-03	1.04e-05	6.35e-03	1.90e-05	1.81e-05	1.84e-02	1.12e-05	1.38e-02	1.82e-05
Chromium (hexavalent)	5.40e-04	NA	NA	4.75e-04	NA	8.71e-04	8.29e-04	NA	5.13e-04	NA	8.34e-04

Table D-2

Bioconcentration Factors for Water to Wildlife Measurement Receptors

(Page 6 of 6)

Compound	Measurement Receptors										
	Muskrat (BCF_{W-OM})	Northern Bobwhite (BCF_{W-OB})	Northern Harrier (BCF_{W-CM})	Red Fox (BCF_{W-CM})	Red-tailed Hawk (BCF_{W-HM})	Salt-marsh Harvest Mouse (BCF_{W-HM})	Short-tailed Shrew (BCF_{W-OM})	Spotted Sandpiper (BCF_{W-CSB})	Swift Fox (BCF_{W-OM})	Western Meadow Lark (BCF_{W-OM})	White-footed Mouse (BCF_{W-OM})
Copper	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Total Cyanide	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lead	2.94e-05	NA	NA	2.59e-05	NA	4.75e-05	4.52e-05	NA	2.80e-05	NA	4.55e-05
Mercuric chloride	5.13e-04	2.61e-03	1.43e-03	4.50e-04	1.43e-03	8.25e-04	7.88e-04	4.16e-03	4.88e-04	3.13e-03	2.99e-03
Methylmercury	7.66e-05	3.90e-04	2.14e-04	6.73e-05	2.14e-04	1.24e-04	1.18e-04	6.23e-04	7.28e-05	4.69e-04	1.18e-04
Nickel	5.89e-04	NA	NA	5.18e-04	NA	9.50e-04	9.04e-04	NA	5.60e-04	NA	9.10e-04
Selenium	2.23e-04	1.24e-01	6.76e-02	1.96e-04	6.76e-02	3.60e-04	3.42e-04	1.96e-01	2.12e-04	1.48e-01	3.44e-04
Silver	2.94e-04	NA	NA	2.59e-04	NA	4.75e-04	4.52e-04	NA	2.80e-04	NA	4.55e-04
Thallium	3.93e-03	NA	NA	3.45e-03	NA	6.34e-03	6.03e-03	NA	3.73e-03	NA	6.07e-03
Zinc	8.83e-06	9.57e-04	5.24e-04	7.77e-06	5.24e-04	1.43e-05	1.36e-05	1.52e-03	8.40e-06	1.14e-03	1.37e-05

Notes:

NA - Indicates insufficient data to determine value

HB - Herbivorous bird
HM - Herbivorous mammal
OB - Omnivorous bird
OM - Omnivorous mammal
TP - Terrestrial plant

– Values provided were determined as specified in the text of Appendix D. *BCF* values for omnivores were determined based on an equal diet. *BCF* values for dioxin and furan congeners determined using BEF values specified in Chapter 2.

TABLE D-3

BIOCONCENTRATION FACTORS FOR SOIL/SEDIMENT TO WILDLIFE MEASUREMENT RECEPTORS

(Page 1 of 6)

Compound	Measurement Receptors										
	American Kestrel (BCF_{S-CB})	American Robin (BCF_{S-OB})	Canvas Back (BCF_{S-HB})	Deer Mouse (BCF_{S-HM})	Least Shrew (BCF_{S-OM})	Long-tailed Weasel (BCF_{S-OM})	Mallard Duck (BCF_{S-OB})	Marsh Rice Rat (BCF_{S-OM})	Marsh Wren (BCF_{S-OB})	Mink (BCF_{S-CM})	Mourning Dove (BCF_{S-OM})
Dioxins and Furans											
2,3,7,8-TCDD	4.78e-01	4.92e+00	6.26e-01	7.81e-05	7.41e-04	1.62e-04	1.09e+00	1.70e-04	6.74e+00	1.05e-04	2.41e+00
1,2,3,7,8-PeCDD	4.40e-01	4.53e+00	5.76e-01	7.19e-05	6.81e-04	1.49e-04	1.01e+00	1.56e-04	6.20e+00	9.66e-05	2.22e+00
1,2,3,4,7,8-HxCDD	1.48e-01	1.53e+00	1.94e-01	2.42e-05	2.30e-04	5.02e-05	3.39e-01	5.26e-05	2.09e+00	3.25e-05	7.48e-01
1,2,3,6,7,8-HxCDD	5.74e-02	5.90e-01	7.51e-02	9.37e-06	8.89e-05	1.94e-05	1.31e-01	2.04e-05	8.09e-01	1.26e-05	2.89e-02
1,2,3,7,8,9-HxCDD	6.69e-02	6.89e-01	8.77e-02	1.09e-05	1.04e-04	2.27e-05	1.53e-01	2.38e-05	9.44e-01	1.47e-05	3.38e-01
1,2,3,4,6,7,8-HpCDD	2.44e-02	2.51e-01	3.19e-02	3.98e-06	3.78e-05	8.26e-06	5.58e-02	8.66e-06	3.44e-01	5.35e-06	1.23e-01
OCDD	5.74e-03	5.90e-02	7.51e-03	9.37e-07	8.89e-06	1.94e-06	1.31e-02	2.04e-06	8.09e-02	1.26e-06	2.89e-02
2,3,7,8-TCDF	3.83e-01	3.94e+00	5.01e-01	6.25e-05	5.93e-04	1.30e-04	8.75e-01	1.36e-04	5.39e+00	8.40e-05	1.93e+00
1,2,3,7,8-PeCDF	1.05e-01	1.08e+00	1.38e-01	1.72e-05	1.63e-04	3.56e-05	2.41e-01	3.74e-05	1.48e+00	2.31e-05	5.31e-01
2,3,4,7,8-PeCDF	7.65e-01	7.87e+00	1.00e+00	1.25e-04	1.19e-03	2.59e-04	1.75e+00	2.72e-04	1.08e+01	1.68e-04	3.86e+00
1,2,3,4,7,8-HxCDF	3.63e-02	3.74e-01	4.76e-02	5.94e-06	5.63e-05	1.23e-05	8.31e-02	1.29e-05	5.12e-01	7.98e-06	1.83e-01
1,2,3,6,7,8-HxCDF	9.09e-02	9.35e-01	1.19e-01	1.48e-05	1.41e-04	3.08e-05	2.08e-01	3.23e-05	1.28e+00	1.99e-05	4.58e-01
2,3,4,6,7,8-HxCDF	3.20e-01	3.30e+00	4.19e-01	5.23e-05	4.96e-04	1.09e-04	7.33e-01	1.14e-04	4.52e+00	7.03e-05	1.62e+00
1,2,3,7,8,9-HxCDF	3.01e-01	3.10e+00	3.94e-01	4.92e-05	4.67e-04	1.02e-04	6.89e-01	1.07e-04	4.25e+00	6.61e-05	1.52e+00
1,2,3,4,6,7,8-HpCDF	5.26e-03	5.41e-02	6.89e-03	8.59e-07	8.15e-06	1.78e-06	1.20e-02	1.87e-06	7.42e-02	1.15e-06	2.65e-02
1,2,3,4,7,8,9-HpCDF	1.86e-01	1.92e+00	2.44e-01	3.05e-05	2.89e-04	6.32e-05	4.27e-01	6.62e-05	2.63e+00	4.09e-05	9.40e-01
OCDF	7.65e-03	7.87e-02	1.00e-02	1.25e-06	1.19e-05	2.59e-06	1.75e-02	2.72e-06	1.08e-01	1.68e-06	3.86e-02
Polynuclear Aromatic Hydrocarbons (PAHs)											
Benzo(a)pyrene	3.71e-05	3.81e-04	4.85e-05	4.86e-05	4.61e-04	1.01e-04	8.50e-05	6.21e-05	5.22e-04	6.53e-05	1.87e-04
Benzo(a)anthracene	1.32e-05	1.35e-04	1.72e-05	1.73e-05	1.64e-04	3.58e-05	3.01e-05	2.20e-05	1.85e-04	2.32e-05	6.63e-05
Benzo(b)fluoranthene	4.39e-05	4.50e-04	5.74e-05	5.75e-05	5.46e-04	1.19e-04	1.01e-04	7.35e-05	6.18e-04	7.73e-05	2.22e-04
Benzo(k)fluoranthene	4.36e-05	4.48e-04	5.71e-05	5.73e-05	5.43e-04	1.19e-04	1.00e-04	7.30e-05	6.14e-04	7.69e-05	2.20e-04
Chrysene	1.52e-05	1.55e-04	1.98e-05	1.99e-05	1.88e-04	4.12e-05	3.47e-05	2.54e-05	2.13e-04	2.67e-05	7.64e-05
Dibenz(a,h)anthracene	9.73e-05	9.98e-04	1.27e-04	1.27e-04	1.21e-03	2.64e-04	2.23e-04	1.63e-04	1.37e-03	1.71e-04	4.91e-04
Indeno(1,2,3-cd)pyrene	2.27e-04	2.32e-03	2.96e-04	2.98e-04	2.82e-03	6.18e-04	5.19e-04	3.79e-04	3.19e-03	4.00e-04	1.14e-03
Polychlorinated Biphenyls (PCBs)											
Aroclor 1016	6.99e-06	7.17e-05	9.14e-06	9.16e-06	8.69e-05	1.90e-05	1.60e-05	1.17e-05	9.83e-05	1.23e-05	3.53e-05
Aroclor 1254	4.43e-05	4.55e-04	5.80e-05	5.83e-05	5.52e-04	1.21e-04	1.02e-04	7.42e-05	6.24e-04	7.83e-05	2.24e-04
Nitroaromatics											
1,3-Dinitrobenzene	8.55e-10	8.77e-09	1.12e-09	1.12e-09	1.06e-08	2.32e-09	1.96e-09	1.43e-09	1.20e-08	1.51e-09	4.31e-09
2,4-Dinitrotoluene	2.72e-09	2.79e-08	3.56e-09	3.58e-09	3.40e-08	7.43e-09	6.24e-09	4.56e-09	3.83e-08	4.81e-09	1.37e-08
2,6-Dinitrotoluene	2.13e-09	2.18e-08	2.78e-09	2.78e-09	2.63e-08	5.76e-09	4.87e-09	3.56e-09	2.99e-08	3.73e-09	1.07e-08

TABLE D-3

BIOCONCENTRATION FACTORS FOR SOIL/SEDIMENT TO WILDLIFE MEASUREMENT RECEPTORS

(Page 2 of 6)

Compound	Measurement Receptors										
	American Kestrel (BCF_{S-CB})	American Robin (BCF_{S-OB})	Canvas Back (BCF_{S-HB})	Deer Mouse (BCF_{S-HM})	Least Shrew (BCF_{S-OM})	Long-tailed Weasel (BCF_{S-OM})	Mallard Duck (BCF_{S-OB})	Marsh Rice Rat (BCF_{S-OM})	Marsh Wren (BCF_{S-OB})	Mink (BCF_{S-CM})	Mourning Dove (BCF_{S-OM})
Nitrobenzene	1.88e-09	1.92e-08	2.45e-09	2.46e-09	2.33e-08	5.10e-09	4.30e-09	3.14e-09	2.64e-08	3.31e-09	9.47e-09
Pentachloronitrobenzene	1.20e-06	1.23e-05	1.57e-06	1.58e-06	1.50e-05	3.28e-06	2.76e-06	2.01e-06	1.69e-05	2.13e-06	6.07e-06
Phthalate Esters											
Bis(2-ethylhexyl)phthalate	4.42e-06	4.53e-05	5.78e-06	5.80e-06	5.50e-05	1.20e-05	1.01e-05	7.40e-06	6.22e-05	7.79e-06	2.23e-05
Di(n)octyl phthalate	5.89e-02	6.04e-01	7.71e-02	7.72e-02	7.32e-01	1.60e-01	1.35e-01	9.86e-02	8.29e-01	1.04e-01	2.97e-01
Volatile Organic Compounds											
Acetone	1.65e-11	1.70e-10	2.16e-11	2.17e-11	2.06e-10	4.51e-11	3.79e-11	2.77e-11	2.33e-10	2.92e-11	8.34e-11
Acrylonitrile	4.91e-11	5.05e-10	6.42e-11	6.43e-11	6.10e-10	1.33e-10	1.12e-10	2.11e-11	6.92e-10	8.64e-11	2.47e-10
Chloroform	2.45e-09	2.51e-08	3.20e-09	3.22e-09	3.06e-08	6.68e-09	5.60e-09	4.09e-09	3.44e-08	4.33e-09	1.23e-08
Crotonaldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
1,4-Dioxane	1.49e-11	1.53e-10	1.94e-11	1.96e-11	1.86e-10	4.06e-11	3.41e-11	2.49e-11	2.09e-10	2.63e-11	7.50e-11
Formaldehyde	6.06e-11	6.21e-10	7.92e-11	7.95e-11	7.54e-10	1.65e-10	1.39e-10	1.01e-10	8.52e-10	1.07e-10	3.06e-10
Vinyl chloride	3.86e-10	3.96e-09	5.05e-10	5.06e-10	4.80e-09	1.05e-09	8.85e-10	6.47e-10	5.44e-09	6.80e-10	1.95e-09
Other Chlorinated Organics											
Hexachlorobenzene	8.77e-06	8.99e-05	1.15e-05	1.15e-05	1.09e-04	2.38e-05	2.01e-05	1.47e-05	1.23e-04	1.54e-05	4.42e-05
Hexachlorobutadiene	1.49e-06	1.53e-05	1.95e-06	1.94e-06	1.84e-05	4.02e-06	3.40e-06	2.49e-06	2.10e-05	2.61e-06	7.50e-06
Hexachlorocyclopentadiene	2.22e-06	2.28e-05	2.91e-06	2.92e-06	2.77e-05	6.06e-06	5.09e-06	3.72e-06	3.13e-05	3.92e-06	1.12e-05
Pentachlorobenzene	3.38e-06	3.46e-05	4.42e-06	4.42e-06	4.19e-05	9.16e-06	7.74e-06	5.65e-06	4.75e-05	5.93e-06	1.70e-05
Pentachlorophenol	3.32e-06	3.41e-05	4.34e-06	4.34e-06	4.12e-05	9.01e-06	7.61e-06	5.56e-06	4.67e-05	5.84e-06	1.68e-05
Pesticides											
4,4-DDE	4.98e-05	5.10e-04	6.51e-05	6.52e-05	6.18e-04	1.35e-04	1.14e-04	8.33e-05	7.00e-04	8.76e-05	2.51e-04
Heptachlor	2.85e-06	2.92e-05	3.73e-06	3.74e-06	3.55e-05	7.76e-06	6.53e-06	4.77e-06	4.01e-05	5.03e-06	1.44e-05
Hexachlorophene	9.56e-04	9.81e-03	1.25e-03	1.25e-03	1.19e-02	2.60e-03	2.19e-03	1.60e-03	1.35e-02	1.68e-03	4.82e-03
Inorganics											
Aluminum	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Antimony	NA	NA	NA	1.44e-06	1.36e-05	2.98e-06	NA	NA	NA	1.93e-06	NA
Arsenic	NA	NA	NA	2.88e-06	2.73e-05	5.97e-06	NA	NA	NA	3.87e-06	NA
Barium	NA	NA	NA	2.16e-07	2.05e-06	4.48e-07	NA	NA	NA	2.90e-07	NA
Beryllium	NA	NA	NA	1.44e-06	1.36e-05	2.98e-06	NA	NA	NA	1.93e-06	NA
Cadmium	1.47e-04	1.51e-03	1.93e-04	1.73e-07	1.64e-06	3.58e-07	3.37e-04	2.47e-04	2.07e-03	2.32e-07	7.43e-04
Chromium (hexavalent)	NA	NA	NA	7.91e-06	7.50e-05	1.64e-05	NA	NA	NA	1.06e-05	NA
Copper	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Total Cyanide	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA

TABLE D-3

BIOCONCENTRATION FACTORS FOR SOIL/SEDIMENT TO WILDLIFE MEASUREMENT RECEPTORS

(Page 3 of 6)

Compound	Measurement Receptors										
	American Kestrel (BCF_{S-CB})	American Robin (BCF_{S-OB})	Canvas Back (BCF_{S-HB})	Deer Mouse (BCF_{S-HM})	Least Shrew (BCF_{S-OM})	Long-tailed Weasel (BCF_{S-OM})	Mallard Duck (BCF_{S-OB})	Marsh Rice Rat (BCF_{S-OM})	Marsh Wren (BCF_{S-OB})	Mink (BCF_{S-CM})	Mourning Dove (BCF_{S-OM})
Lead	NA	NA	NA	4.32e-07	4.09e-06	8.95e-07	NA	NA	NA	5.80e-07	NA
Mercuric chloride	3.32e-05	3.42e-04	4.35e-05	7.52e-06	7.10e-05	1.56e-05	7.60e-05	5.57e-05	4.68e-04	1.01e-05	1.68e-04
Methylmercury	4.98e-06	5.12e-05	6.52e-06	1.12e-06	1.06e-05	2.33e-06	1.14e-05	8.34e-06	7.02e-05	1.51e-06	2.51e-05
Nickel	NA	NA	NA	8.63e-06	8.18e-05	1.79e-05	NA	NA	NA	1.16e-05	NA
Selenium	1.57e-03	1.61e-02	2.05e-03	3.27e-06	3.10e-05	6.77e-06	3.60e-03	2.63e-03	2.21e-02	4.39e-06	7.92e-03
Silver	NA	NA	NA	4.32e-06	4.09e-05	8.95e-06	NA	NA	NA	5.80e-06	NA
Thallium	NA	NA	NA	5.75e-05	5.46e-04	1.19e-04	NA	NA	NA	7.73e-05	NA
Zinc	1.22e-05	1.25e-04	1.59e-05	1.29e-07	1.23e-06	2.69e-07	2.79e-05	2.04e-05	1.71e-04	1.74e-07	6.13e-05

Notes:

NA - Indicates insufficient data to determine value

HB - Herbivorous bird
HM - Herbivorous mammal
OB - Omnivorous bird
OM - Omnivorous mammal
S - Soil/Sediment

– Values provided were determined as specified in the text of Appendix D. *BCF* values for omnivores were determined based on an equal diet. *BCF* values for dioxin and furan congeners determined using BEF values specified in Chapter 2.

TABLE D-3

BIOCONCENTRATION FACTORS FOR SOIL/SEDIMENT TO WILDLIFE MEASUREMENT RECEPTORS

(Page 4 of 6)

	Measurement Receptors										
Compound	**Muskrat (BCF_{S-OM})**	**Northern Bobwhite (BCF_{S-OB})**	**Northern Harrier (BCF_{S-CM})**	**Red Fox (BCF_{S-CM})**	**Red-tailed Hawk (BCF_{S-HM})**	**Salt-marsh Harvest Mouse (BCF_{S-HM})**	**Short-tailed Shrew (BCF_{S-OM})**	**Spotted Sandpiper (BCF_{S-CSB})**	**Swift Fox (BCF_{S-OM})**	**Western Meadow Lark (BCF_{S-OM})**	**White-footed Mouse (BCF_{S-OM})**
Dioxins and Furans											
2,3,7,8-TCDD	3.48e-05	4.13e+00	3.42e+00	8.19e-05	3.42e+00	9.66e-05	7.41e-04	1.43e+01	9.41e-05	4.78e+00	1.47e-04
1,2,3,7,8-PeCDD	3.20e-05	3.80e+00	3.15e+00	7.53e-05	3.15e+00	8.88e-05	6.81e-04	1.31e+01	8.66e-05	4.40e+00	1.35e-04
1,2,3,4,7,8-HxCDD	1.08e-05	1.28e+00	1.06e+00	2.54e-05	1.06e+00	2.99e-05	2.30e-04	4.43e+00	2.92e-05	1.48e+00	4.55e-05
1,2,3,6,7,8-HxCDD	4.18e-07	4.95e-01	4.11e-01	9.82e-06	4.11e-01	1.16e-05	8.89e-05	1.71e+00	1.13e-05	5.74e-01	1.76e-05
1,2,3,7,8,9-HxCDD	4.87e-06	5.78e-01	4.79e-01	1.15e-05	4.79e-01	1.35e-05	1.04e-04	2.00e+00	1.32e-05	6.69e-01	2.05e-05
1,2,3,4,6,7,8-HpCDD	1.78e-06	2.11e-01	1.75e-01	4.17e-06	1.75e-01	4.92e-06	3.78e-05	7.28e-01	4.80e-06	2.44e-01	7.48e-06
OCDD	4.18e-07	4.95e-02	4.11e-02	9.82e-07	4.11e-02	1.16e-06	8.89e-06	1.71e-01	1.13e-06	5.74e-02	1.76e-06
2,3,7,8-TCDF	2.79e-05	3.30e+00	2.74e+00	6.55e-05	2.74e+00	7.72e-05	5.93e-04	1.14e+01	7.53e-05	3.83e+00	1.17e-04
1,2,3,7,8-PeCDF	7.66e-06	9.08e-01	7.53e-01	1.80e-05	7.53e-01	2.12e-05	1.63e-04	3.14e+00	2.07e-05	1.05e+00	3.23e-05
2,3,4,7,8-PeCDF	5.57e-05	6.60e+00	5.48e+00	1.31e-04	5.48e+00	1.55e-04	1.19e-03	2.28e+01	1.51e-04	7.65e+00	2.35e-04
1,2,3,4,7,8-HxCDF	2.65e-06	3.14e-01	2.60e-01	6.22e-06	2.60e-01	7.34e-06	5.63e-05	1.09e+00	7.15e-06	3.63e-01	1.12e-05
1,2,3,6,7,8-HxCDF	6.62e-06	7.84e-01	6.50e-01	1.56e-05	6.50e-01	1.83e-05	1.41e-04	2.71e+00	1.79e-05	9.09e-01	2.79e-05
2,3,4,6,7,8-HxCDF	2.33e-05	2.77e+00	2.29e+00	5.48e-05	2.29e+00	6.47e-05	4.96e-04	9.56e+00	6.30e-05	3.20e+00	9.83e-05
1,2,3,7,8,9-HxCDF	2.19e-05	2.60e+00	2.16e+00	5.16e-05	2.16e+00	6.08e-05	4.67e-04	8.99e+00	5.93e-05	3.01e+00	9.24e-05
1,2,3,4,6,7,8-HpCDF	3.83e-07	4.54e-02	3.77e-02	9.00e-07	3.77e-02	1.06e-06	8.15e-06	1.57e-01	1.04e-06	5.26e-02	1.61e-06
1,2,3,4,7,8,9-HpCDF	1.36e-05	1.61e+00	1.33e+00	3.19e-05	1.33e+00	0.00e+00	2.89e-04	5.57e+00	3.67e-05	1.86e+00	5.72e-05
OCDF	5.57e-07	6.60e-02	5.48e-02	1.31e-06	5.48e-02	1.55e-06	1.19e-05	2.28e-01	1.51e-06	7.65e-02	2.35e-06
Polynuclear aromatic hydrocarbons (PAHs)											
Benzo(a)pyrene	2.17e-05	3.19e-04	2.66e-04	5.10e-05	2.66e-04	6.01e-05	4.61e-04	1.11e-03	5.86e-05	3.72e-04	9.13e-05
Benzo(a)anthracene	7.69e-06	1.13e-04	9.41e-05	1.81e-05	9.41e-05	2.13e-05	1.64e-04	3.93e-04	2.08e-05	1.32e-04	3.24e-05
Benzo(b)fluoranthene	2.57e-05	3.78e-04	3.14e-04	6.03e-05	3.14e-04	7.11e-05	5.46e-04	1.31e-03	6.93e-05	4.40e-04	1.08e-04
Benzo(k)fluoranthene	2.55e-05	3.75e-04	3.12e-04	6.00e-05	3.12e-04	7.08e-05	5.43e-04	1.30e-03	6.90e-05	4.37e-04	1.08e-04
Chrysene	8.85e-06	1.30e-04	1.08e-04	2.08e-05	1.08e-04	2.45e-05	1.88e-04	4.53e-04	2.39e-05	1.52e-04	3.73e-05
Dibenz(a,h)anthracene	5.68e-05	8.37e-04	6.97e-04	1.34e-04	6.97e-04	1.58e-04	1.21e-03	2.91e-03	1.54e-04	9.75e-04	2.39e-04
Indeno(1,2,3-cd)pyrene	1.33e-04	1.95e-03	1.62e-03	3.12e-04	1.62e-03	3.68e-04	2.82e-03	6.77e-03	3.59e-04	2.27e-03	5.59e-04
Polychlorinated biphenyls (PCBs)											
Aroclor 1016	4.08e-06	6.01e-05	5.01e-05	9.60e-06	5.01e-05	1.13e-05	8.69e-05	2.09e-04	1.10e-05	7.01e-05	1.72e-05
Aroclor 1254	2.60e-05	3.81e-04	3.17e-04	6.11e-05	3.17e-04	7.20e-05	5.52e-04	1.32e-03	7.02e-05	4.44e-04	1.09e-04
Nitroaromatics											
1,3-Dinitrobenzene	5.00e-10	7.35e-09	6.12e-09	1.17e-09	6.12e-09	1.39e-09	1.06e-08	2.55e-08	1.35e-09	8.57e-09	2.10e-09
2,4-Dinitrotoluene	1.60e-09	2.34e-08	1.95e-08	3.75e-09	1.95e-08	4.43e-09	3.40e-08	8.14e-08	4.32e-09	2.73e-08	6.73e-09

TABLE D-3

BIOCONCENTRATION FACTORS FOR SOIL/SEDIMENT TO WILDLIFE MEASUREMENT RECEPTORS

(Page 5 of 6)

	Measurement Receptors										
Compound	**Muskrat (BCF_{S-OM})**	**Northern Bobwhite (BCF_{S-OB})**	**Northern Harrier (BCF_{S-CM})**	**Red Fox (BCF_{S-CM})**	**Red-tailed Hawk (BCF_{S-HM})**	**Salt-marsh Harvest Mouse (BCF_{S-HM})**	**Short-tailed Shrew (BCF_{S-OM})**	**Spotted Sandpiper (BCF_{S-CSB})**	**Swift Fox (BCF_{S-OM})**	**Western Meadow Lark (BCF_{S-OM})**	**White-footed Mouse (BCF_{S-OM})**
2,6-Dinitrotoluene	1.24e-09	1.83e-08	1.52e-08	2.91e-09	1.52e-08	3.43e-09	2.63e-08	6.35e-08	3.34e-09	2.13e-08	5.21e-09
Nitrobenzene	1.10e-09	1.61e-08	1.34e-08	2.58e-09	1.34e-08	3.04e-09	2.33e-08	5.61e-08	2.96e-09	1.88e-08	4.62e-09
Pentachloronitrobenzene	7.05e-07	1.04e-05	8.62e-06	1.66e-06	8.62e-06	1.96e-06	1.50e-05	3.60e-05	1.91e-06	1.21e-05	2.97e-06
Phthalate esters											
Bis(2-ethylhexyl)phthalate	2.58e-06	3.80e-05	3.16e-05	6.07e-06	3.16e-05	7.17e-06	5.50e-05	1.32e-04	6.98e-06	4.43e-05	1.09e-05
Di(n)octyl phthalate	3.44e-02	5.07e-01	4.22e-01	8.09e-02	4.22e-01	9.55e-02	7.32e-01	1.76e+00	9.31e-02	5.91e-01	1.45e-01
Volatile organic compounds											
Acetone	9.68e-12	1.42e-10	1.18e-10	2.28e-11	1.18e-10	2.69e-11	2.06e-10	4.94e-10	2.62e-11	1.66e-10	4.08e-11
Acrylonitrile	2.87e-11	4.42e-10	3.51e-11	6.74e-11	3.51e-10	7.95e-11	6.10e-10	1.46e-09	7.75e-11	4.91e-10	1.21e-10
Chloroform	1.44e-09	2.10e-08	1.75e-08	3.38e-09	1.75e-08	3.98e-09	3.06e-08	7.31e-08	3.88e-09	2.45e-08	6.05e-09
Crotonaldehyde	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
1,4-Dioxane	8.72e-12	1.28e-10	1.06e-10	2.05e-11	1.06e-10	2.42e-11	1.86e-10	4.44e-10	2.36e-11	1.49e-10	3.67e-11
Formaldehyde	3.55e-11	5.21e-10	4.34e-10	8.34e-11	4.34e-10	9.83e-11	7.54e-10	1.81e-09	9.58e-11	6.07e-10	1.49e-10
Vinyl chloride	2.26e-10	3.32e-09	2.77e-09	5.31e-10	2.77e-09	6.26e-10	4.80e-09	1.15e-08	6.10e-10	3.87e-09	9.51e-10
Other chlorinated organics											
Hexachlorobenzene	5.12e-06	7.54e-05	6.28e-05	1.20e-05	6.28e-05	1.42e-05	1.09e-04	2.62e-04	1.38e-05	8.79e-05	2.16e-05
Hexachlorobutadiene	8.65e-07	1.28e-05	1.06e-05	2.04e-06	1.06e-05	2.40e-06	1.84e-05	4.44e-05	2.34e-06	1.49e-05	3.65e-06
Hexachlorocyclopentadiene	1.30e-06	1.91e-05	1.59e-05	3.06e-06	1.59e-05	3.61e-06	2.77e-05	6.64e-05	3.52e-06	2.23e-05	5.49e-06
Pentachlorobenzene	1.97e-06	2.90e-05	2.42e-05	4.63e-06	2.42e-05	5.46e-06	4.19e-05	1.01e-04	5.32e-06	3.39e-05	8.30e-06
Pentachlorophenol	1.94e-06	2.86e-05	2.38e-05	4.55e-06	2.38e-05	5.37e-06	4.12e-05	9.93e-05	5.23e-06	3.33e-05	8.16e-06
Pesticides											
4,4-DDE	2.90e-05	4.28e-04	3.56e-04	6.83e-05	3.56e-04	8.06e-05	6.18e-04	1.49e-03	7.85e-05	4.99e-04	1.22e-04
Heptachlor	1.67e-06	2.45e-05	2.04e-05	3.92e-06	2.04e-05	4.62e-06	3.55e-05	8.51e-05	4.51e-06	2.86e-05	7.03e-06
Hexachlorophene	5.59e-04	8.22e-03	6.85e-03	1.31e-03	6.85e-03	1.55e-03	1.19e-02	2.86e-02	1.51e-03	9.58e-03	2.35e-03
Inorganics											
Aluminum	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Antimony	6.41e-07	NA	NA	1.51e-06	NA	1.78e-06	1.36e-05	NA	1.73e-06	NA	2.70e-06
Arsenic	1.28e-06	NA	NA	3.01e-06	NA	3.56e-06	2.73e-05	NA	3.47e-06	NA	5.40e-06
Barium	9.62e-08	NA	NA	2.26e-07	NA	2.67e-07	2.05e-06	NA	2.60e-07	NA	4.05e-07
Beryllium	6.41e-07	NA	NA	1.51e-06	NA	1.78e-06	1.36e-05	NA	1.73e-06	NA	2.70e-06
Cadmium	7.69e-08	1.27e-03	1.05e-03	1.81e-07	1.05e-03	2.13e-07	1.64e-06	4.40e-03	2.08e-07	1.48e-03	3.24e-07
Chromium (hexavalent)	3.53e-06	NA	NA	8.29e-06	NA	9.78e-06	7.50e-05	NA	9.53e-06	NA	1.49e-05

TABLE D-3

BIOCONCENTRATION FACTORS FOR SOIL/SEDIMENT TO WILDLIFE MEASUREMENT RECEPTORS

(Page 6 of 6)

	Measurement Receptors										
Compound	**Muskrat (BCF_{S-OM})**	**Northern Bobwhite (BCF_{S-OB})**	**Northern Harrier (BCF_{S-CM})**	**Red Fox (BCF_{S-CM})**	**Red-tailed Hawk (BCF_{S-HM})**	**Salt-marsh Harvest Mouse (BCF_{S-HM})**	**Short-tailed Shrew (BCF_{S-OM})**	**Spotted Sandpiper (BCF_{S-CSB})**	**Swift Fox (BCF_{S-OM})**	**Western Meadow Lark (BCF_{S-OM})**	**White-footed Mouse (BCF_{S-OM})**
Copper	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Total Cyanide	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lead	1.92e-07	NA	NA	4.52e-07	NA	5.33e-07	4.09e-06	NA	5.20e-07	NA	8.11e-07
Mercuric chloride	3.35e-06	2.87e-04	2.38e-04	7.88e-06	2.38e-04	9.29e-06	7.10e-05	9.92e-04	9.03e-06	3.32e-04	1.41e-05
Methylmercury	5.00e-07	4.30e-05	3.56e-05	1.18e-06	3.56e-05	1.39e-06	1.06e-05	1.49e-04	1.35e-06	4.98e-05	2.11e-06
Nickel	3.85e-06	NA	NA	9.04e-06	NA	1.07e-05	8.18e-05	NA	1.04e-05	NA	1.62e-05
Selenium	1.46e-06	1.35e-02	1.12e-02	3.42e-06	1.12e-02	4.04e-06	3.10e-05	4.69e-02	3.93e-06	1.57e-02	6.13e-06
Silver	1.92e-06	NA	NA	4.52e-06	NA	5.33e-06	4.09e-05	NA	5.20e-06	NA	8.11e-06
Thallium	2.57e-05	NA	NA	6.03e-05	NA	7.11e-05	5.46e-04	NA	6.93e-05	NA	1.08e-04
Zinc	5.77e-08	1.05e-04	8.71e-05	1.36e-07	8.71e-05	1.60e-07	1.23e-06	3.63e-04	1.56e-07	1.22e-04	2.43e-07

Notes:

NA - Indicates insufficient data to determine value

HB - Herbivorous bird
HM - Herbivorous mammal
OB - Omnivorous bird
OM - Omnivorous mammal
S - Soil/Sediment

– Values provided were determined as specified in the text of Appendix D. *BCF* values for omnivores were determined based on an equal diet. *BCF* values for dioxin and furan congeners determined using BEF values specified in Chapter 2.

APPENDIX E

TOXICITY REFERENCE VALUES

Screening Level Ecological Risk Assessment Protocol

August 1999

APPENDIX E

TABLE OF CONTENTS

APPENDIX E

TOXICITY REFERENCE VALUES

Appendix E presents implementation of the recommended approach (described in Chapter 5) for identifying toxicity reference values (*TRV*s) for measurement receptors. Discussion is provided for determining compound-specific *TRV* values for community and wildlife measurement receptors.

Following the guidance in Sections E-1.0 through E-1.2, U.S. EPA OSW has identified default *TRV* values for the measurement receptors of the seven example food webs (listed in Chapter 4) and the compounds commonly identified in ecological risk assessments for combustion facilities (identified in Chapter 2). Section E-1.0 describes the determination of *TRV* values for surface water, sediment, and soil community measurement receptors in the example food webs. Section E-2.0 describes determination of *TRV* values for wildlife measurement receptors in the example food webs. Tables E-1 through E-8 present the default *TRV* values selected, the basis for selection of each value, and the references evaluated in determination of each value.

TRV values for a limited number of compounds are included in this appendix (see Tables E-1 through E-3) to facilitate the completion of screening ecological risk assessments. However, it is expected that *TRV* values for additional compounds and receptors may be required for evaluation on a site specific basis. In such cases, *TRV* values for these additional compounds could be determined following the same guidance used in determination of the *TRV* values reported in this appendix. For the determination of *TRV* values for measurement receptors not specifically represented in Sections E-1.0 through E-2.0 (e.g., amphibians and reptiles), an approach consistent to that presented in this appendix could be utilized by applying data applicable to those measurement receptors being evaluated.

The default *TRV*s provided in Tables E-1 through E-8 are based on values reported in available scientific literature. Toxicity values identified in secondary reference sources were verified, where possible, by reviewing the primary reference source. As noted in Chapter 5, *TRV* values may change as additional toxicity research is conducted and the availability of toxicity data in the scientific literature increases. As a result, U.S. EPA OSW recommends evaluating the latest toxicity data before completing a risk assessment to ensure that the toxicity data used in the risk assessment is the most current. If more appropriate *TRV* values can be documented, they should be used presented to the respective permitting authority for approval.

*TRV*s were not identified for amphibians and reptiles because of the paucity of toxicological information on these receptors. Additional guidance on determination and use of *TRV* values in the screening level ecological risk assessment is provided in Chapter 5.

E-1.0 *TRVs* FOR COMMUNITY MEASUREMENT RECEPTORS IN SURFACE WATER, SEDIMENT, AND SOIL

TRV values provided in this appendix for community measurement receptors in surface water, sediment, and soil were identified from screening toxicity values developed and/or adopted by federal and/or state regulatory agencies. As discussed in Chapter 5, these screening toxicity values are generally provided in the form of standards, criteria, guidance, or benchmarks. For compounds with no available screening toxicity value, *TRV*s were determined using toxicity values from available scientific literature. The

equilibrium partitioning (EqP) approach was used to compute several sediment *TRV*s. Uncertainty factors (UFs) were applied to toxicity values, as necessary, to meet the *TRV* criteria discussed in Chapter 5. The following sections discuss determination of *TRV* values for community receptors in surface water, sediment, and soil.

Freshwater TRVs Freshwater *TRV*s should be used for freshwater and estuarine ecosystems with a salinity less than 5 parts per thousand. Freshwater *TRV*s, based on the dissolved concentration of the compound in surface water, are listed in Table E-1. *TRV*s were identified using the following hierarchy:

1. Federal chronic ambient water quality criteria (AWQC) calculated for with no final residue value (U.S. EPA 1999; 1996b). Federal AWQC for cadmium, copper, lead, nickel, and zinc were multiplied by a chemical-specific conversion factor to determine a *TRV* based on dissolved concentration (U.S. EPA 1999; 1996b).

2. Final chronic values (FCV) for COPCs for which their AWQC included a final residue value (U.S. EPA 1996b).

3. If inadequate data (insufficient number of families of aquatic life with toxicity data) were available to compute an AWQC or FCV, U.S. EPA (1999; 1996b) also reported secondary chronic values (SCV) calculated using the Tier II method in the Great Lakes Water Quality Initiative (GLWQI) (reported in 40 CFR Part 122). This method is similar to the procedures for calculating an FCV. It uses statistically-derived "adjustment factors" to address deficiencies in available data. The adjustment factor decreases as the number of representative families increases.

4. If an AWQC, FCV, or GLWQI Tier II SCV value were not available, toxicity values cited by U.S. EPA (1987) were identified. These toxicity values represent the lowest available values. Further, additional toxicity values available from the AQUIRE database in U.S. EPA's *ECOTOXicology Database System* (U.S. EPA 1996a) were identified. If collected from a secondary source (such as AQUIRE), original studies were obtained and reviewed for accuracy. The toxicity values reported in Table E-1 represent the lowest (most conservative), ecologically relevant, available value.

5. If toxicity data were unavailable, a surrogate *TRV* from a COPC with a similar structure was identified.

6. If no surrogate was available, a *TRV* was not listed. The potential toxicity of a COPC with no *TRV* should be addressed as an uncertainty (see Chapter 6)

Standard AQUIRE report summaries on tests were screened for duration, endpoint, effect, and concentration. Studies were also screened for ecologically relevant effects by focusing on studies that evaluated effects on survival, reproduction, and growth. Aspects of endpoint, duration, and test organism in each toxicity study were evaluated to identify the most appropriate study. Several compounds, most notably metals, had a large number of toxicity values based on various endpoints, organisms, and exposure durations. In these instances, best scientific judgment was used to identify the most appropriate toxicity value (see Chapter 5).

Chronic NOAEL-based values were not adjusted, but rather were carried through unchanged to become the *TRV*. Toxicity values identified as "less than" a particular concentration were divided by 2 to represent an average value because the true value is unknown, and it occurs between 0 and the noted concentration. *UF*s discussed in Chapter 5 were applied to toxicity values not meeting *TRV* criteria.

Saltwater TRVs Saltwater *TRV*s are applicable to marine water bodies and estuarine systems with a salinity greater than 5 ppt. Saltwater *TRV*s are listed in Table E-2. Saltwater water *TRV* development followed the same procedure as described above for freshwater receptors, except no GLWQI Tier II SCVs were available. In addition, if no saltwater *TRV* for a surrogate compound was available, the corresponding freshwater *TRV* was adopted.

Freshwater Sediment TRVs Freshwater sediment *TRV*s are listed in Table E-3. They are applicable to water bodies with a salinity less than 5 ppt. Freshwater sediment *TRV*s were identified from various sets of screening values and ecotoxicity review documents. The lowest available screening values among the following sources were identified:

1. No effect level (NEL) and lowest effect level (LEL) values from "Ontario's Approach to Sediment Assessment and Remediation" (Persaud et al. 1993)

2. Apparent effects threshold (AET) values for the amphipod, *Hyallela azteca*, reported in "Creation of Freshwater Sediment Quality Database and Preliminary Analysis of Freshwater Apparent Effects Thresholds" (Washington State Department of Ecology 1994)

3. Sediment effect concentrations jointly published by the National Biological Service and the U.S. EPA (Ingersoll et al. 1996).

If a screening value was not available in the sources listed above, toxicity studies and other values compiled and reported by Jones, Hull, and Suter (1997) were reviewed to identify possible *TRV*s. Relevant studies were prioritized based on the criteria listed in Chapter 5, and uncertainty factors were applied, as applicable, based on criteria presented (see Chapter 5).

If a screening or sediment toxicity value was not available for an organic COPC, a freshwater sediment *TRV* was computed, using the EqP approach (see Chapter 5), from the compounds corresponding freshwater *TRV* and K_{oc} value. The U.S. EPA Office of Water utilizes the EqP approach to develop sediment quality criteria for nonionic (neutral) organic chemicals (U.S. EPA 1993). The EqP approach assumes that the toxicity of a compound in sediment is a function of the concentration in pore water and that to be nontoxic, the pore water must meet the surface water final chronic value. The EqP approach also assumes that the concentration of a compound in sediment pore water depends on the carbon content of the sediment and the compound's organic carbon partitioning coefficient (U.S. EPA 1993). A *TRV* may be calculated using the following equation (U.S. EPA 1993):

$$TRV_{sed} = K_{oc} \cdot f_{oc} \cdot TRV_{sw} \qquad \text{Equation E-1}$$

where

TRV_{sed} = Sediment *TRV* (µg/kg)

K_{oc} = Organic carbon partition coefficient (L/kg)
f_{oc} = Fraction of organic carbon in sediment (unitless)—default value = 4% (0.04)
TRV_{sw} = Corresponding surface water *TRV* (µg/L)

Marine Sediment TRVs Marine sediment *TRV*s are listed in Table E-4. They are applicable to sediments of marine water bodies and estuarine systems with a salinity greater than 5 ppt. Marine sediment *TRV*s were developed following the procedures used to identify the freshwater sediment *TRV*s. Screening values were compiled from the following sources:

1. No observed effect level (NOEL) sediment quality assessment guidelines for State of Florida coastal waters (MacDonald 1993).

2. Marine and estuarine effects range low (ERL) values from "Incidence of Adverse Biological Effects Within Ranges of Chemical Concentrations in Marine and Estuarine Sediments" (Long et al. 1995)

3. ERL values from "The Potential for Biological Effects of Sediment-Sorbed Contaminants Tested in the National Status and Trends Program" (Long and Morgan 1991)

4. Marine sediment quality criteria from "Sediment Management Standards" (Washington State Department of Ecology 1991)

Screening values were adopted directly as *TRV*s. If a screening value was not available in the sources listed above, toxicity values from a search of the scientific literature and those compiled and reported by Hull and Suter (1994) were reviewed to identify possible *TRV*s. Original studies were obtained, where possible, and toxicity values were verified. Relevant studies were prioritized based on the criteria listed in Chapter 5, and uncertainty factors were applied, as appropriate, based on criteria (see Chapter 5). If a screening or ecologically relevant sediment toxicity value from the scientific literature were not available for an organic COPC, a marine sediment *TRV* was computed, using the EqP approach, from the COPC's corresponding saltwater *TRV* and K_{oc} value (see Equation E-1).

Terrestrial Plant TRVs The terrestrial plant *TRV*s listed in Table E-5 are based on bulk soil exposures. Available terrestrial plant toxicity values from the scientific literature were used to develop presented *TRV* values. Toxicity values were first identified from the following secondary sources:

1. Studies cited in *Toxicological Benchmarks for Screening Potential Contaminants of Concern for Effects on Terrestrial Plants: 1997 Revision* (Efroymson, Will, Suter, and Wooten 1997). Available studies were obtained and reviewed for accuracy of toxicity values. UFs were applied depending on study endpoint and available information.

2. Toxicity values in the Phytotox database in U.S. EPA's *ECOTOXicology Database* System. Available studies were obtained and toxicity values were verified. UFs were applied depending on study endpoint and available information.

3. Toxicity values in U.S. EPA Region 5 *Ecological Data Quality Levels (EDQL) Database* (PRC 1995). The database contains media-specific EDQLs for the RCRA Appendix IX constituents (40 CFR Part 264). The EDQLs represent conservative media concentrations

protective of media receptors and wildlife that might be exposed through food chains based in these media. Available studies were obtained and toxicity values were verified. UFs were applied depending on study endpoint and available information.

Original studies were obtained, where possible, and prioritized based on criteria listed in Chapter 5. Uncertainty factors were applied, as appropriate, based on criteria (discussed in Chapter 5) to develop *TRV* values. For COPCs without toxicity data, the *TRV* for a surrogate COPC was adopted. If an appropriate surrogate *TRV* was not available, no *TRV* value was identified. Generally, review of toxicity data available in the scientific literature indicates that limited *TRV*s are available for organic compounds; while *TRV*s for metals are available.

Soil Invertebrate TRVs The soil invertebrate *TRV*s listed in Table E-6 are based on bulk soil exposures. Available soil invertebrate toxicity values from the scientific literature were used to develop *TRV*s for these receptors. Soil invertebrate toxicity values were first identified from the following secondary sources:

1. Studies cited in *Toxicological Benchmarks for Potential Contaminants of Concern for Effects on Soil and Litter Invertebrates and Heterotrophic Process* (Will and Suter II 1995a). Available studies were obtained and toxicity values were verified. UFs were applied depending on study endpoint and available information.

2. Scientific literature was searched for toxicity values for outstanding compounds. Relevant studies were obtained, toxicity values were verified, and UFs were applied as described.

Original studies were obtained, where possible, and prioritized based on criteria listed in Chapter 5. Uncertainty factors were applied, as appropriate, based on criteria to develop *TRV*s. If no toxicity value was available for a COPC, the *TRV* for a surrogate COPC was adopted.

E-2.0 *TRVs* FOR WILDLIFE MEASUREMENT RECEPTORS

TRV values for wildlife measurement receptors are listed in Tables E-7 (mammals) and E-8 (birds). *TRV*s were not developed for each avian and mammalian measurement receptor in the seven example food webs because of the paucity of species-specific data. Rather, U.S. EPA OSW focused on identifying a set of avian *TRV*s and a set of mammalian *TRV*s for the classes of compounds listed in Section 2.3. U.S. EPA OSW assumed that, among the literature reviewed for a particular guild, the lowest available toxicity value across orders in class Aves and across orders in class Mammalia would provide a conservative estimate of toxicity. Available mammalian and avian toxicity values from the scientific literature were used to develop *TRV*s for these receptors. Also, as previously noted, *TRV* values were not identified for amphibians and reptiles because of the paucity of toxicological information on these receptors. Wildlife measurement receptors *TRV* values were first identified from the following secondary sources:

1. Toxicity values compiled in *Toxicological Benchmarks for Wildlife: 1996 Revision* (Sample, Opresko, and Suter 1996).

2. Toxicity values listed in the Terretox database of U.S. EPA's *ECOTOXicology Database System* (U.S. EPA 1996b) were screened to identify studies potentially meeting the criteria listed in Chapter 5.

Original studies were compiled, where possible, and reviewed to verify their accuracy based on criteria listed in Chapter 5. In many cases, best scientific judgement was used to screen out studies with poor experimental design (see Chapter 5). Uncertainty factors were applied, as appropriate, to develop *TRVs* based on criteria presented in Chapter 5.

Conversions Some avian and mammalian toxicity data are expressed in terms of compound concentration in the food of the test organism. To convert to daily dose, it is necessary to determine the exposure duration and organism body weight. If the study does not report this information, the results should not be used to compute a *TRV*. If information on exposure duration and organism body weight is available, dietary concentration can be computed to dose using the following generic equation:

$$DD = \frac{C \cdot IR}{BW} \qquad \text{Equation E-2}$$

where

DD	=	COPC dose (mg COPC/kg BW/day)
C	=	Concentration of COPC in diet (mg COPC/kg food)
IR	=	Food ingestion rate (kg/day)
BW	=	Test organism body weight (kg)

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TABLES OF TOXICITY REFERENCE (*TRV*) VALUES

Screening Level Ecological Risk Assessment Protocol

August 1999

TABLE E-1

FRESHWATER TOXICITY REFERENCE VALUES

(Page 1 of 8)

Compound	Toxicity Value		Uncertainty Factor[b]	TRV[c]	Reference and Notes [d]
	Duration and Endpoint[a]	Concentration			
Polychlorinateddibenzo-p-dioxins (μg/L)					
2,3,7,8-TCDD	Chronic LOEL	0.000038	0.1	0.0000038	Mehrle et al. (1988). 2,3,7,8-TCDD toxicity value for rainbow trout (*Oncorhynchus mykiss*).
Polynuclear aromatic hydrocarbons (PAH) (μg/L)					
Total high molecular weight (HMW) PAHs	--	--	--	0.014	Benzo(a)pyrene toxicity used as surrogate measure of toxicity. This TRV should be used if assessing the risk of total HMW PAHs.
Benzo(a)pyrene	Tier II value	0.014	Not applicable	0.014	U.S. EPA (1996). Calculated using Great Lakes Water Quality Initiative Tier II methodology.
Benzo(a)anthracene	Tier II SCV	0.027	Not applicable	0.027	Suter and Tsao (1996). Calculated using Great Lakes Water Quality Initiative Tier II methodology.
Benzo(b)fluoranthene	--	--	--	0.027	Toxicity value not available. Benzo(a)anthracene used as surrogate.
Benzo(k)fluoranthene	--	--	--	0.027	Toxicity value not available. Benzo(a)anthracene used as surrogate.
Chrysene	--	--	--	0.027	Toxicity value not available. Benzo(a)anthracene used as surrogate.
Dibenz(a,h)anthracene	--	--	--	0.027	Toxicity value not available. Benzo(a)anthracene used as surrogate.
Indeno(1,2,3-cd)pyrene	--	--	--	0.027	Toxicity value not available. Benzo(a)anthracene used as surrogate.
Polychlorinated biphenyls (PCB) (μg/L)					
Aroclor 1016	--	0.19	Not applicable	0.19	Adopted from U.S. EPA (1996) value for Total PCB. Calculated using Great Lakes Water Quality Initiative Tier II methodology.

TABLE E-1

FRESHWATER TOXICITY REFERENCE VALUES

(Page 2 of 8)

Compound	Toxicity Value		Uncertainty Factor[b]	TRV[c]	Reference and Notes [d]
	Duration and Endpoint[a]	Concentration			
Aroclor 1254	--	0.19	Not applicable	0.19	Adopted from U.S. EPA (1996) value for Total PCB. Calculated using Great Lakes Water Quality Initiative Tier II methodology.
Nitroaromatics (μg/L)					
1,3-Dinitrobenzene	Subchronic NOEC	260	0.1	26	van der Schalie (1983). Algal growth test with *Selenastrum capricornutum.*
2,4-Dinitrotoluene	Chronic LOEL	230	0.1	23	U.S. EPA (1987)
2,6-Dinitrotoluene	Chronic NOEC	60	Not applicable	60	Kuhn et al. (1989). Toxicity value for water flea (*Daphnia magna*).
Nitrobenzene	Acute LOEL	27,000	0.01[e]	270	U.S. EPA (1987)
Pentachloronitrobenzene	LC50	1,000	0.01	10	Hashimoto and Nishiuchi (1981). Toxicity value for common carp (*Cyprinus carpio*).
Phthalate esters (μg/L)					
Bis(2-ethylhexyl)phthalate	Tier II SCV	3.0	Not applicable	3.0	Suter and Tsao (1996). Calculated using Great Lakes Water Quality Initiative Tier II methodology.
Di(n)octyl phthalate	Chronic NOEL	320	Not applicable	320	McCarthy and Whitmore (1985). Toxicity value for water flea (*D. magna*).
Volatile organic compounds (μg/L)					
Acetone	Tier II SCV	1,500	Not applicable	1,500	Suter and Tsao (1996). Calculated using Great Lakes Water Quality Initiative Tier II methodology.
Acrylonitrile	Chronic LOEL	2,600	0.1	260	U.S. EPA (1987)
Chloroform	Tier II SCV	28	Not applicable	28	Suter and Tsao (1996). Calculated using Great Lakes Water Quality Initiative Tier II methodology.

TABLE E-1

FRESHWATER TOXICITY REFERENCE VALUES

(Page 3 of 8)

Compound	Toxicity Value		Uncertainty Factor[b]	TRV[c]	Reference and Notes [d]
	Duration and Endpoint[a]	Concentration			
Crotonaldehyde	Acute LC50	3,500	0.01	35	Dawson et al. (1977). Toxicity value for bluegill sunfish (*Lepomis macrochirus*).
1,4-Dioxane	Acute EC0	6,210,000	0.01	62,100	Bringmann and Kühn (1982). Toxicity value for water flea (*D. magna*).
Formaldehyde	Acute LC50	4,960	0.01	49.6	Reardon and Harrell (1990). No data available for formalehyde. Formalin containing 37 percent formaldehyde used as a surrogate. Endpoint based on formaldehyde concentration.
Vinyl chloride	Subchronic LC100	388,000	0.01[e]	3,880	Brown et al. (1977)
Other chlorinated organics (μg/L)					
Hexachlorobenzene	Proposed chronic criterion	3.68	Not applicable	3.68	U.S. EPA (1987)
Hexachlorobutadiene	Chronic LOEL	9.3	0.1	0.93	U.S. EPA (1987)
Hexachlorocyclopentadiene	Chronic LOEL	5.2	0.1	0.52	U.S. EPA (1987)
Pentachlorobenzene	Tier II value	0.47	Not applicable	0.47	U.S. EPA (1996). Calculated using Great Lakes Water Quality Initiative Tier II methodology.
Pentachlorophenol	Chronic criterion	15	Not applicable	15	U.S. EPA (1999). Value expressed as a function of pH and calculated as follows: TRV = exp(1.005(pH)-5.134). A pH of 7.8 is assumed to calculate the displayed value.
Pesticides (μg/L)					
4,4'-DDE	Acute LOEL	1,050	0.01[e]	10.5	U.S. EPA (1987)
Heptachlor	Chronic criterion	0.0038	Not applicable	0.0038	U.S. EPA (1987)

TABLE E-1

FRESHWATER TOXICITY REFERENCE VALUES

(Page 4 of 8)

Compound	Toxicity Value		Uncertainty Factor[b]	TRV[c]	Reference and Notes [d]
	Duration and Endpoint[a]	Concentration			
Hexachlorophene	Subchronic NOEC	8.8	0.1	0.88	Call et al. (1989). Toxicity value for fathead minnow (*P. promelas*).
Inorganics (mg/L) [f]					
Aluminum	FCV	0.087	Not applicable	0.087	U.S. EPA (1988)
Antimony	Proposed chronic criterion	0.03	Not applicable	0.03	U.S. EPA (1987)
Arsenic (trivalent)	Chronic criterion	0.15	Not applicable	0.15	U.S. EPA (1999)
Barium	Tier II SCV	0.004	Not applicable	0.004	Suter and Tsao (1996). Calculated using Great Lakes Water Quality Initiative Tier II methodology.
Beryllium	Tier II SCV	0.00066	Not applicable	0.00066	Suter and Tsao (1996). Calculated using Great Lakes Water Quality Initiative Tier II methodology.
Cadmium	Chronic criterion	0.0022 (dissolved)	Not applicable	0.0022	U.S. EPA (1999). Value expressed as a function of water hardness and calculated as follows: TRV = $\exp(m_c[\ln(\text{hardness})]+b_c)$ where $m_c = 0.7852$ and $b_c = -2.715$. Criterion was converted to dissolved concentration using the following conversion factor: 1.101672-[(ln hardness)(0.041838]. A assumed hardness of 100 mg/L and a conversion from mg/L to μg/L were used to calculate the displayed value.
Chromium (hexavalent)	Chronic criterion	0.011	Not applicable	0.011	U.S. EPA (1999).
Copper	Chronic criterion	0.009 (dissolved)	Not applicable	0.009	U.S. EPA (1999). Value expressed as a function of water hardness and calculated as follows: TRV = $\exp(m_c[\ln(\text{hardness})]+b_c)$ where $m_c = 0.8545$ and $b_c = -1.702$. Criterion was converted to dissolved concentration using a conversion factor of 0.960. A assumed hardness of 100 mg/L and a conversion from mg/L to μg/L were used to calculate the displayed value.

TABLE E-1

FRESHWATER TOXICITY REFERENCE VALUES

(Page 5 of 8)

Compound	Toxicity Value		Uncertainty Factor[b]	TRV[c]	Reference and Notes [d]
	Duration and Endpoint[a]	Concentration			
Total Cyanide	Chronic criterion	0.0052	Not applicable	0.0052	U.S. EPA (1999). This value is expressed as mg free cyanide (as CN)/L.
Lead	Chronic criterion	0.0025 (dissolved)	Not applicable	0.0025	U.S. EPA (1999). Value expressed as a function of water hardness and calculated as follows: TRV = $\exp(m_c[\ln(\text{hardness})]+b_c)$ where $m_c = 1.273$ and $b_c = -4.705$. Criterion was converted to dissolved concentration using the following conversion factor: 1.46203-[(ln hardness)(0.145712]. A assumed hardness of 100 mg/L and a conversion from mg/L to μg/L were used to calculate the displayed value.
Mercuric chloride	Chronic criterion	0.00077	Not applicable	0.00077	U.S. EPA (1999). This value was from data for inorganic mercury (II).
Methyl mercury	Tier II SCV	0.0000028	Not applicable	0.0000028	Suter and Tsao (1996). Calculated using Great Lakes Water Quality Initiative Tier II methodology.
Nickel	Chronic criterion	0.052 (dissolved)	Not applicable	0.052	U.S. EPA (1999). Value expressed as a function of water hardness and calculated as follows: TRV = $\exp(m_c[\ln(\text{hardness})]+b_c)$ where $m_c = 0.8460$ and $b_c = 0.0584$. Criterion was converted to dissolved concentration using a conversion factor of 0.997. A assumed hardness of 100 mg/L and a conversion from mg/L to μg/L were used to calculate the displayed value.
Selenium	Chronic criterion	0.005	Not applicable	0.005	U.S. EPA (1999)
Silver	Proposed chronic criterion	0.00012	Not applicable	0.00012	U.S. EPA (1987)
Thallium	Chronic LOEL	0.04	0.1	0.004	U.S. EPA (1987)

TABLE E-1

FRESHWATER TOXICITY REFERENCE VALUES

(Page 6 of 8)

Compound	Toxicity Value		Uncertainty Factor[b]	TRV[c]	Reference and Notes [d]
	Duration and Endpoint[a]	Concentration			
Zinc	Chronic criterion	0.118 (dissolved)	Not applicable	0.118	U.S. EPA (1999). Value expressed as a function of water hardness and calculated as follows: TRV = $\exp(m_c[\ln(\text{hardness})]+b_c)$ where $m_c = 0.8473$ and $b_c = 0.884$. Criterion was converted to dissolved concentration using a conversion factor of 0.986. A assumed hardness of 100 mg/L and a conversion from mg/L to μg/L were used to calculate the displayed value.

Notes:

a The duration of exposure is defined as chronic if it represents about 10 percent or more of the test animals lifetime expectancy. Acute exposures represent single exposures or multiple exposures occurring within a short time. For evaluating exposure duration, the following general guidelines were used. For invertebrates and other lower trophic level aquatic biota: (1) chronic duration lasted for 7 or more days, (2) subchronic duration lasted from 3 to 6 days, and (3) acute duration lasted 2 days or less. For fish: (1) chronic duration lasted for more than 90 days, (2) subchronic duration lasted from 14 to 90 days, and (3) acute duration lasted less than 2 weeks.

b Uncertainty factors are used to extrapolate a toxicity value to a chronic NOAEL TRV. See Chapter 5 (Section 5.4) of the SLERAP for a discussion of the use of uncertainty factors.

c TRV was calculated by multiplying the toxicity value with the uncertainty factor.

d The references refer to the source of the toxicity value. Complete reference citations are provided below.

e Best scientific judgment used to identify uncertainty factor. See Chapter 5 (Section 5.4.1.2) for a discussion the use of best scientific judgement. Factors evaluated include test duration, ecological relevance of endpoint, experimental design, and availability of toxicity data.

f TRVs for metals are based on the dissolved metal concentration. According to U.S. EPA (1993) policy, concentrations of dissolved metal more closely approximate the bioavailable fraction of metal in the water column.

EC0 = Effective concentration for zero percent of the test organisms.
FCV = Final Chronic Value
HMW = High molecular weight
LC50 = Lethal concentration for 50 percent of the test organisms.
LC100 = Lethal concentration for 100 percent of the test organisms.
LOEL = Lowest Observed Effect Level
NOEC = No Observed Effect Concentration
NOEL = No Observed Effect Level
SCV = Secondary Chronic Value
TRV = Toxicity Reference Value

TABLE E-1

FRESHWATER TOXICITY REFERENCE VALUES

(Page 7 of 8)

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TABLE E-2

MARINE/ESTUARINE SURFACE WATER TOXICITY REFERENCE VALUES

(Page 1 of 8)

Compound	Toxicity Value		Uncertainty Factor[b]	Toxicity Reference Value[c]	Reference and Notes [d]
	Duration and Endpoint[a]	Concentration			
Polychlorinateddibnzo-p-dioxins (μg/L)					
2,3,7,8-TCDD	LOEC	0.000038	0.1	0.0000038	No saltwater data were available, therefore, corresponding freshwater toxicity value was used (rainbow trout, *Oncorhynchus mykiss*) from Mehrle et al. (1988). 2,3,4,5-TCDD toxicity value used.
Polynuclear aromatic hydrocarbons (PAH) (μg/L)					
Total high molecular weight (HMW) PAHs	Acute LC50	>50	0.01[e]	0.5	Rossi and Neff (1978) evaluated toxicity of three HMW (three or more aromatic rings) PAHs to the polychaete, *Neanthes arenaceodentata*. LC50 of each HMW PAH exceeded 50 μg/L. This TRV should be used if assessing the risk of total HMW PAHs.
Benzo(a)pyrene	Acute LC50	>50	0.01[e]	0.5	Rossi and Neff (1978). Toxicity value for polychaete (*N. arenaceodentata*).
Benzo(a)anthracene	Acute LC50	>50	0.01[e]	0.5	Toxicity value not available. TRV for benzo(a)pyrene used as surrogate.
Benzo(b)fluoranthene	Acute LC50	>50	0.01[e]	0.5	Toxicity value not available. TRV for benzo(a)pyrene used as surrogate.
Benzo(k)fluoranthene	Acute LC50	>50	0.01[e]	0.5	Toxicity value not available. TRV for benzo(a)pyrene used as surrogate.
Chrysene	Acute LC50	>50	0.01[e]	0.5	Rossi and Neff (1978). Toxicity of several PAHs was evaluted. LC50 of each individual HMW PAH exceeded 50 μg/L.
Dibenz(a,h)anthracene	Acute LC50	>50	0.01[e]	0.5	Rossi and Neff (1978). Toxicity of several PAHs was evaluted. LC50 of individual HMW PAHs exceeded 50 μg/L.
Indeno(1,2,3-cd)pyrene	Acute LC50	>50	0.01[e]	0.5	Toxicity value not available. TRV for benzo(a)pyrene used as surrogate.
Polychlorinated biphenyls (PCB) (μg/L)					
Aroclor 1016	--	0.03	Not applicable	0.03	U.S. EPA (1987) chronic criterion for ambient water quality.

TABLE E-2

MARINE/ESTUARINE SURFACE WATER TOXICITY REFERENCE VALUES

(Page 2 of 8)

Compound	Toxicity Value		Uncertainty Factor[b]	Toxicity Reference Value[c]	Reference and Notes [d]
	Duration and Endpoint[a]	Concentration			
Aroclor 1254	--	0.03	Not applicable	0.03	U.S. EPA (1987) chronic criterion for ambient water quality.
Nitroaromatics (μg/L)					
1,3-Dinitrobenzene	--	--	--	66.8	Toxicity data not available. TRV for nitrobenzene used as surrogate.
2,4-Dinitrotoluene	Chronic criterion	370	Not applicable	370	U.S. EPA (1987)
2,6-Dinitrotoluene	--	--	--	370	Toxicity data not available. TRV for 2,4-dinitrotoluene used as surrogate.
Nitrobenzene	Acute criterion	6,680	0.01	66.8	U.S. EPA (1987)
Pentachloronitrobenzene	Acute LC50	1,000	0.01	10	No toxicity value or surrogate TRV available, therefore, corresponding freshwater toxicity value (common carp, *Cyprinus carpio*) from Hashimoto and Nishiuchi (1981) adopted.
Phthalate esters (μg/L)					
Bis(2-ethylhexyl)phthalate	Acute LC50	>170	0.01	1.7	Adams et al. (1995). Toxicity value for sheepshead minnow (*Cyprinodon variegatus*).
Di(n)octyl phthalate	NOEL	320	Not applicable	320	No toxicity value or surrogate TRV available, therefore, corresponding freshwater toxicity value used (water flea, *D. magna*) from McCarthy and Whitmore (1985).
Volatile organic compounds (μg/L)					
Acetone	Acute LC50	2,100,000	0.01	21,000	Price et al. (1974). Toxicity value for brine shrimp (*Artemia* sp.).
Acrylonitrile	Acute LC50	10,000	0.01	100	Portmann and Wilson (1971). Toxicity value for common shrimp (*Crangon crangon*).

TABLE E-2

MARINE/ESTUARINE SURFACE WATER TOXICITY REFERENCE VALUES

(Page 3 of 8)

Compound	Toxicity Value		Uncertainty Factor[b]	Toxicity Reference Value[c]	Reference and Notes [d]
	Duration and Endpoint[a]	Concentration			
Chloroform	Acute LC 50	18,000	0.01	180	Anderson and Luster (1980). Toxicity value for Rainbow trout (*Salmo gairdnari*).
Crotonaldehyde	Acute LC50	1,300	0.01	13	Dawson et al. (1977). Toxicity value for inland silverside (*Menidia beryllina*).
1,4-Dioxane	Acute LC50	6,700,000	0.01	67,000	Dawson et al. (1977). Toxicity value for inland silverside (*M. beryllina*).
Formaldehyde	Acute LC50	4,960	0.01	49.6	No toxicity value or surrogate TRV available for this constituent, therefore, corresponding freshwater toxicity value used (Striped bass, *Morone saxatilis*) from Reardon and Harell (1990). No data available for formadehyde. Formalin containing 37 percent formaldehyde used as surrogate. TRV expressed on formaldehyde basis.
Vinyl chloride	Subchronic LC100	388,000	0.01[e]	3,880	No toxicity value of surrogate TRV available, therefore, corresponding freshwater toxicity value used (Northern pike, *Esox lucius*) from Brown et al. (1977).
Other chlorinated organics (μg/L)					
Hexachlorobenzene	Acute EC50	>1,000	0.01	10	Zaroogian (1981). Toxicity value for American oyster (*Crassostrea virginica*).
Hexachlorobutadiene	Acute LOEL	32	0.01[e]	0.32	U.S. EPA (1987)
Hexachlorocyclopentadiene	Acute LOEL	7.0	0.01[e]	0.07	U.S. EPA (1987)
Pentachlorobenzene	Subchronic NOEC	18	0.1	1.8	Hansen and Cripe (1991). Toxicity value for sheepshead minnow (*Cyprinodon variegatus*).
Pentachlorophenol	Chronic criterion	7.9	Not applicable	7.9	U.S. EPA (1987)
Pesticides (μg/L)					

TABLE E-2

MARINE/ESTUARINE SURFACE WATER TOXICITY REFERENCE VALUES

(Page 4 of 8)

Compound	Toxicity Value		Uncertainty Factor[b]	Toxicity Reference Value[c]	Reference and Notes [d]
	Duration and Endpoint[a]	Concentration			
4,4'-DDE	Acute LOEL	14	0.01[e]	0.14	U.S. EPA (1987)
Heptachlor	Chronic criterion	0.0036	Not applicable	0.0036	U.S. EPA (1987)
Hexachlorophene	Acute LC50	3.3	0.01	0.033	Calleja et al. (1994). Toxicity value for brine shrimp (*Artemia salina*).
Inorganics (mg/L)					
Aluminum	Acute LT50	0.271	0.01	0.00271	Study examined influence of pH and temperature on acute (48-hour) toxicity (as time to mortality) of aluminum to smoltifying Atlantic salmon (*Salmo salar*). Endpoint concentration based on sum of inorganic and organic aluminum for exposure at pH 6.5 (Poleo and Muniz 1993).
Antimony	Proposed chronic criterion	0.5	Not applicable	0.5	U.S. EPA (1987)
Arsenic (trivalent)	Chronic criterion	0.036	Not applicable	0.036	U.S. EPA (1987)
Barium	Subchronic LC50	>500.	0.01[e]	5.0	U.S. EPA (1978)
Beryllium	Tier II SCV	0.00066	Not applicable	0.00066	No toxicity value or surrogate TRV available, therefore, corresponding freshwater TRV adopted. Suter and Tsao (1996); value calculated using Great Lakes Water Quality Initiative Tier II methodology.
Cadmium	Chronic criterion	0.0093	Not applicable	0.0093	U.S. EPA (1987)
Chromium (hexavalent)	Chronic criterion	0.05	Not applicable	0.05	U.S. EPA (1987)
Copper	Chronic criterion	0.0031	Not applicable	0.0031	U.S. EPA 1999. When the concentration of dissolved organic carbon is elevated, copper is substantially less toxic and use of a water effects ratio may be appropriate.

TABLE E-2

MARINE/ESTUARINE SURFACE WATER TOXICITY REFERENCE VALUES

(Page 5 of 8)

Compound	Toxicity Value		Uncertainty Factor[b]	Toxicity Reference Value[c]	Reference and Notes [d]
	Duration and Endpoint[a]	Concentration			
Total Cyanide	Chronic criterion	0.001	Not applicable	0.001	U.S. EPA (1987)
Lead	Chronic criterion	0.0081	Not applicable	0.0081	U.S. EPA (1999)
Mercuric chloride	Chronic criterion	0.00094	Not applicable	0.00094	U.S. EPA (1999). This value was from data for inorganic mercury (II).
Methyl mercury	Subchronic NOAEL	0.030	0.1	0.003	Sharp and Neff (1982). Toxicity value for mummichog (*Fundulus heteroclitus*).
Nickel	Chronic criterion	0.0082	Not applicable	0.0082	U.S. EPA (1999)
Selenium	Chronic criterion	0.071	Not applicable	0.071	U.S. EPA (1987)
Silver	Chronic criterion/ proposed criterion	0.0023	Not applicable	0.0023	U.S. EPA (1987)
Thallium	Acute LOEL	2.13	0.01[e]	0.02	U.S. EPA (1987)
Zinc	Chronic criterion	0.081	1.0	0.081	U.S. EPA (1999)

TABLE E-2

MARINE/ESTUARINE SURFACE WATER TOXICITY REFERENCE VALUES

(Page 6 of 8)

Notes:

a The duration of exposure is defined as chronic if it represents about 10 percent or more of the test animals lifetime expectancy. Acute exposures represent single exposures or multiple exposures occurring within a short time. For evaluating exposure duration, the following general guidelines were used. For invertebrates and other lower trophic level aquatic biota: (1) chronic duration lasted for 7 or more days, (2) subchronic duration lasted from 3 to 6 days, and (3) acute duration lasted 2 days or less. For fish: (1) chronic duration lasted for more than 90 days, (2) subchronic duration lasted from 14 to 90 days, and (3) acute duration lasted less than 2 weeks.

b Uncertainty factors are used to extrapolate a toxicity value to a chronic NOAEL TRV. See Chapter 5 (Section 5.4) of the SLERAP for a discussion of the use of uncertainty factors.

c TRV was calculated by multiplying the toxicity value with the uncertainty factor.

d The references refer to the source of the toxicity value. Complete reference citations are provided at the end of this appendix.

e Best scientific judgment used to identify uncertainty factor. See Chapter 5 (Section 5.4.1.2) for a discussion of the use of best scientific judgement. Factors evaluated include test duration, ecological relevance of endpoint, experimental design, and availability of toxicity data.

EC50 = Effective concentration for 50 percent of the test organisms.
FCV = Final Chronic Values
HMV = High molecular weight
LC50 = Lethal concentration for 50 percent of the test organisms.
LC100 = Lethal concentration for 100 percent of the test organisms.
LOEC = Lowest Observed Effect Concentration
LOEL = Lowest Observed Effect Level
LT50 = Lethal threshold concentration for 50 percent of the test organisms.
NOAEL = No Observed Adverse Effect Level
NOEL = No Observed Effect Level
SCV = Secondary Chronic Value
TRV = Toxicity Reference Value

TABLE E-2

MARINE/ESTUARINE SURFACE WATER TOXICITY REFERENCE VALUES

(Page 7 of 8)

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TABLE E-3

FRESHWATER SEDIMENT TOXICITY REFERENCE VALUES

(Page 1 of 7)

Compound	Freshwater TRV [a]	K_{oc} Value [b]	Bed Sediment TRV (dry weight)	Reference and Notes [c]
Polychlorinateddibenzo-p-dioxins (μg/kg)				
2,3,7,8-TCDD	0.0000038	2,691,535	0.41	TRV was calculated using equilibrium partitioning (EqP) approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Polynuclear aromatic hydrocarbons (PAH) (μg/kg)				
Total high molecular weight (HMW) PAH	Not applicable	Not applicable	170	TRV is ERL value computed by Ingersoll et al. (1996) based on 28-day amphipod (*Hyalella azteca*) toxicity tests. This TRV may be used if risk of total HMW PAHs is assessed.
Benzo(a)pyrene	Not applicable	Not applicable	84	TRV is an ERL value calculated by Ingersoll et al. (1996) based on 28-day *H. azteca* toxicity tests.
Benzo(a)anthracene	Not applicable	Not applicable	19	TRV is an ERL value calculated by Ingersoll et al. (1996) based on 28-day *H. azteca* toxicity tests.
Benzo(b)fluoranthene	Not applicable	Not applicable	37	TRV is an ERL value calculated by Ingersoll et al. (1996) based on 28-day *H. azteca* toxicity tests.
Benzo(k)fluoranthene	Not applicable	Not applicable	37	TRV is an ERL value calculated by Ingersoll et al. (1996) based on 28-day *H. azteca* toxicity tests.
Chrysene	Not applicable	Not applicable	30	TRV is an ERL value calculated by Ingersoll et al. (1996) based on 28-day *H. azteca* toxicity tests.
Dibenz(a,h)anthracene	Not applicable	Not applicable	10	TRV is an ERL value calculated by Ingersoll et al. (1996) based on 28-day *H. azteca* toxicity tests.
Indeno(1,2,3-cd)pyrene	Not applicable	Not applicable	30	TRV is an ERL value calculated by Ingersoll et al. (1996) based on 28-day *H. azteca* toxicity tests.

TABLE E-3

FRESHWATER SEDIMENT TOXICITY REFERENCE VALUES

(Page 2 of 7)

Compound	Freshwater TRV [a]	K_{oc} Value [b]	Bed Sediment TRV (dry weight)	Reference and Notes [c]
Polychlorinated biphenyls (PCB) (μg/kg)				
Aroclor 1016	Not applicable	Not applicable	50	TRV is an ERL value for Total PCB calculated by Ingersoll et al. (1996) based on 28-day *H. azteca* toxicity tests.
Aroclor 1254	Not applicable	Not applicable	50	TRV is an ERL value for Total PCB calculated by Ingersoll et al. (1996) based on 28-day *H. azteca* toxicity tests.
Nitroaromatics (μg/kg)				
1,3-Dinitrobenzene	26	20.6	21.4	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
2,4-Dinitrotoluene	23	51	46.9	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
2,6-Dinitrotoluene	60	41.9	100.6	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Nitrobenzene	270	119	1285.2	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Pentachloronitrobenzene	10	5,890	2356	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Phthalate esters (μg/kg)				
Bis(2-ethylhexyl)phthalate	3	111,000	1.33×10^{4}	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Di(n)octyl phthalate	320	9.03×10^{8}	1.16×10^{10}	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]

TABLE E-3

FRESHWATER SEDIMENT TOXICITY REFERENCE VALUES

(Page 3 of 7)

Compound	Freshwater TRV [a]	K_{oc} Value [b]	Bed Sediment TRV (dry weight)	Reference and Notes [c]
Volatile organic compounds (μg/kg)				
Acetone	1,500	0.951	57.1	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Acrylonitrile	260	2.22	23.1	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Chloroform	28	53.0	59.4	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Crotonaldehyde	35	Not available	Not calculated	No TRV was calculated because no K_{oc} or K_{ow} values were identified for this constituent.
1,4-Dioxane	62,100	0.876	2176.0	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Formaldehyde	49.6	2.62	5.2	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Vinyl chloride	3,880	11.1	1722.7	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Other chlorinated organics (μg/kg)				
Hexachlorobenzene	Not applicable	Not applicable	20	TRV is an LEL value (Persaud et al. 1993).
Hexachlorobutadiene	0.93	6,940	258.2	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Hexachlorocyclopentadiene	0.52	9,510	197.8	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]

TABLE E-3

FRESHWATER SEDIMENT TOXICITY REFERENCE VALUES

(Page 4 of 7)

Compound	Freshwater TRV [a]	K_{oc} Value [b]	Bed Sediment TRV (dry weight)	Reference and Notes [c]
Pentachlorobenzene	0.47	32,148	604.4	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Pentachlorophenol	Not applicable	Not applicable	7,000	TRV is an AET value for *H. azteca* (Washington State Department of Ecology 1994).
Pesticides (μg/kg)				
4,4'-DDE	Not applicable	Not applicable	5	TRV is an LEL value (Persaud et al. 1993). p,p'-DDE used as a surrogate.
Heptachlor	Not applicable	Not applicable	0.3	TRV is an NEL value (Persaud et al. 1993). The NEL was selected because no LEL was available.
Hexachlorophene	0.88	1,800,000	63,360	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Inorganics (mg/kg)				
Aluminum	Not applicable	Not applicable	14,000	TRV is an ERL value calculated by Ingersoll et al. (1996) based on 28-day *H. azteca* toxicity tests.
Antimony	Not applicable	Not applicable	64.0	TRV is an AET for *H. azteca* (Washington State Department of Ecology 1994).
Arsenic	Not applicable	Not applicable	6.0	TRV is an LEL value (Persaud et al. 1993).
Barium	Not applicable	Not applicable	20	TRV is a U.S. EPA Region 5 guideline value for classification of sediments for determining the suitability of dredged sediments for open water disposal, as cited in Hull and Suter II (1994).
Beryllium	Not applicable	Not applicable	Not available	Regulatory or toxicity value not available.
Cadmium	Not applicable	Not applicable	0.6	TRV is an LEL value (Persaud et al. 1993).

TABLE E-3

FRESHWATER SEDIMENT TOXICITY REFERENCE VALUES

(Page 5 of 7)

Compound	Freshwater TRV [a]	K_{oc} Value [b]	Bed Sediment TRV (dry weight)	Reference and Notes [c]
Chromium (total)	Not applicable	Not applicable	26	TRV is an LEL value (Persaud et al. 1993).
Copper	Not applicable	Not applicable	16	TRV is an LEL value (Persaud et al. 1993).
Total Cyanide	Not applicable	Not applicable	0.1	TRV is a U.S. EPA Region 5 guideline value for classification of sediments for determining the suitability of dredged sediments for open water disposal, as cited in Hull and Suter II (1994).
Lead	Not applicable	Not applicable	31	TRV is an LEL value (Persaud et al. 1993).
Mercuric chloride	Not applicable	Not applicable	0.2	No toxicity data available for divalent inorganic mercury. Total mercury used as surrogate for divalent inorganic mercury. TRV is an LEL value (Persaud et al. 1993).
Methyl mercury	Not applicable	Not applicable	0.2	No toxicity data available for methyl mercury. Total mercury used as surrogate for methylmercury. TRV is an LEL value (Persaud et al. 1993).
Nickel	Not applicable	Not applicable	16	TRV is an LEL value (Persaud et al. 1993).
Selenium	Not applicable	Not applicable	0.1	TRV is an AET for *H. azteca* (Washington State Department of Ecology 1994).
Silver	Not applicable	Not applicable	4.5	TRV is an AET for *H. azteca* (Washington State Department of Ecology 1994).
Thallium	Not applicable	Not applicable	Not available	Regulatory value or toxicity value not available.
Zinc	Not applicable	Not applicable	110	TRV is an ERL value calculated by Ingersoll et al. (1996) based on 28-day *H. azteca* toxicity tests.

TABLE E-3

FRESHWATER SEDIMENT TOXICITY REFERENCE VALUES

(Page 6 of 7)

Notes:

a Toxicity reference values are in units of micrograms per kilogram (μg/kg) and milligrams per kilograms (mg/kg) for organic and inorganic constituents, respectively.

b Values are in units of liters per kilogram (L/kg). K_{oc} = Organic carbon normalized sorption coefficient. References and equations used to calculate K_{oc} values are provided in Appendix A.

c The references refer to the study from which the TRV was identified. Complete reference citations are provided below.

d Freshwater sediment TRV calculated with the following equation:

$$\text{Freshwater sediment TRV} = \text{Freshwater TRV (Table E-1)} * K_{oc} * f_{oc,bs}$$

where,

K_{oc} = organic carbon partition coefficient, and

$f_{oc,bs}$= fraction of organic carbon in bed sediment, assumed to be 4 percent = 0.04.

K_{oc} values discussed in Appendix A.

AET = Apparent Effects Threshold
ERL = Effects Range-Low
EqP = Equilibrium Partitioning
HMV = High molecular weight
LEL = Lowest Effect Level
NEL = No Effect Level
TRV = Toxicity Reference Value

TABLE E-3

FRESHWATER SEDIMENT TOXICITY REFERENCE VALUES

REFERENCES

Default TRVs for sediments in freshwater habitats were identified from the three sets of freshwater toxicity values presented below. While some compound-specific freshwater sediment toxicity information is available in the scientific literature, available toxicity values were not used because of the compexity in understanding the role of naturally-occurring sediment features (such as grain size, ammonia, sulfide, soil type, and organic carbon content) in toxicity to benthic invertebrates. Among these sets of value, the lowest available toxicity value for a particular compound was adopted as the TRV. In many cases, a default TRV was calculated from the corresponding freshwater TRV using EPA's equilibrium partitioning approach, assuming a 4 percent organic carbon content.

Hull, R.N. and G.W. Suter II. 1994. *Toxicological Benchmarks for Screening Contaminants of Potential Concern for Effects on Sediment-Associated Biota: 1994 Revision.* ES/ER/TM-95/R1. Environmental Sciences Division, Oak Ridge National Laboratory. Oak Ridge, Tennessee. June.

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Washington State Department of Ecology. 1991. *Sediment Management Standards*. Washington Administrative Code 173-204.

Washington State Department of Ecology. 1994. *Creation and Analysis of Freshwater Sediment Quality Values in Washington State*. Publication No. 97-32-a. July.

TABLE E-4

MARINE/ESTUARINE SEDIMENT TOXICITY REFERENCE VALUES

(Page 1 of 8)

Compound	Marine/Estuarine Surface Water TRV[a]	K_{oc} Value[b]	Bed Sediment TRV (dry weight)	Reference and Notes [c]
Ploychlorinateddibenzo-p-dioxins (μg/kg)				
2,3,7,8-TCDD	0.0000038	2,691,535	0.41	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Polynuclear aromatic hydrocarbons (PAH) (μg/kg)				
Total high molecular weight (HMW) PAH	Not applicable	Not applicable	870	Recommended NOEL for Florida Department of Environmental Regulation (DER) (MacDonald 1993). This TRV may be used in risk of total HMW PAHs is assessed.
Benzo(a)pyrene	Not applicable	Not applicable	230	Recommended NOEL for Florida DER (MacDonald 1993).
Benzo(a)anthracene	Not applicable	Not applicable	160	Recommended NOEL for Florida DER (MacDonald 1993).
Benzo(b)fluoranthene	0.5	836,000	418,000	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Benzo(k)fluoranthene	Not applicable	Not applicable	240	TRV is a LEL value from Persaud et al. (1993).
Chrysene	Not applicable	Not applicable	220	Recommended NOEL for Florida DER (MacDonald 1993).
Dibenz(a,h)anthracene	Not applicable	Not applicable	31	Recommended NOEL for Florida DER (MacDonald 1993).
Indeno(1,2,3-cd)pyrene	Not applicable	Not applicable	1,360	TRV was computed from OC-based marine sediment quality criterion from Washington State Department of Ecology (1991) and fractional organic carbon content of 0.04, as follows: TRV = 34 mg/kg * 0.04 * 1000 μg/mg.

TABLE E-4

MARINE/ESTUARINE SEDIMENT TOXICITY REFERENCE VALUES

(Page 2 of 8)

Compound	Marine/Estuarine Surface Water TRV[a]	K_{oc} Value[b]	Bed Sediment TRV (dry weight)	Reference and Notes [c]
Polychlorinated biphenyls (PCB) (μg/kg)				
Aroclor 1016	Not applicable	Not applicable	22.7	TRV is an ERL value for Total PCB from Long et al. (1995).
Aroclor 1254	Not applicable	Not applicable	22.7	TRV is an ERL value for Total PCB from Long et al. (1995).
Nitroaromatics (μg/kg)				
1,3-Dinitrobenzene	66.8	20.6	55.0	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
2,4-Dinitrotoluene	370	51	754.8	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
2,6-Dinitrotoluene	370	41.9	620.1	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Nitrobenzene	66.8	119	318.0	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Pentachloronitrobenzene	10	5,890	2356	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]

TABLE E-4

MARINE/ESTUARINE SEDIMENT TOXICITY REFERENCE VALUES

(Page 3 of 8)

Compound	Marine/Estuarine Surface Water TRV[a]	K_{oc} Value[b]	Bed Sediment TRV (dry weight)	Reference and Notes [c]
Phthalate esters (μg/kg)				
Bis(2-ethylhexyl)phthalate	Not applicable	Not applicable	470	TRV was calculated using OC-based marine sediment quality criterion from Washington State Department of Ecology (1991) and fractional organic carbon content of 0.04, as follows: TRV = 47 mg/kg * 0.04 * 1000 μg/mg.
Di(n)octyl phthalate	Not applicable	Not applicable	580	TRV was calculated using OC-based marine sediment quality criterion from Washington State Department of Ecology (1991) and fractional organic carbon content of 0.04, as follows: TRV = 58 mg/kg * 0.04 * 1000 μg/mg.
Volatile organic compounds (μg/kg)				
Acetone	21,000	0.951	798.8	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Acrylonitrile	100	2.22	8.88	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Chloroform	180	53.0	381.6	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Crotonaldehyde	13	Not available	Not computed	No TRV was calculated because no K_{oc} or K_{ow} value was identified.
1,4-Dioxane	67,000	0.876	2348	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Formaldehyde	49.6	2.62	5.2	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]

TABLE E-4

MARINE/ESTUARINE SEDIMENT TOXICITY REFERENCE VALUES

(Page 4 of 8)

Compound	Marine/Estuarine Surface Water TRV[a]	K_{oc} Value[b]	Bed Sediment TRV (dry weight)	Reference and Notes [c]
Vinyl chloride	3,880	11.1	1722.7	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Other chlorinated organics (μg/kg)				
Hexachlorobenzene	Not applicable	Not applicable	15.2	TRV was calculated using OC-based marine sediment quality criterion from Washington State Department of Ecology (1991) and a fractional OC content of 0.04, as follows: TRV = 0.38 mg/kg * 0.04 * 1000 μg/mg.
Hexachlorobutadiene	Not applicable	Not applicable	156	TRV was calculated using OC-based marine sediment quality criterion from Washington State Department of Ecology (1991) and a fractional OC content of 0.04, as follows: TRV = 3.9 mg/kg * 0.04 * 1000 μg/mg.
Hexachlorocyclopentadiene	0.07	9,510	26.6	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Pentachlorobenzene	1.8	32,148	2315	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Pentachlorophenol	Not applicable	Not applicable	360	TRV is marine sediment quality criterion from Washington State Department of Ecology (1991).
Pesticides (μg/kg)				
4,4'-DDE	Not applicable	Not applicable	1.7	Recommended NOEL for p,p'-DDE for Florida DER (MacDonald 1993).
Heptachlor	0.0036	9,530	1.37	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]
Hexachlorophene	0.033	1,800,000	2376	TRV was calculated using EqP approach (EPA 1993), assuming a fractional organic content of 0.04. [d]

TABLE E-4

MARINE/ESTUARINE SEDIMENT TOXICITY REFERENCE VALUES

(Page 5 of 8)

Compound	Marine/Estuarine Surface Water TRV[a]	K_{oc} Value[b]	Bed Sediment TRV (dry weight)	Reference and Notes [c]
Inorganics (mg/kg)				
Aluminum	Not applicable	Not applicable	Not available	Screening or toxicity value not available.
Antimony	Not applicable	Not applicable	2	TRV is an ERL value (Long and Morgan 1991).
Arsenic	Not applicable	Not applicable	6	TRV is an LEL value for Province of Ontario (Persaud et al. 1993).
Barium	Not applicable	Not applicable	20	TRV is a U.S. EPA Region 5 guideline value for classification of sediments for determining the suitability of dredged material for open water disposal, as cited in Hull and Suter II (1994).
Beryllium	Not applicable	Not applicable	Not available	Screening or toxicity value not available.
Cadmium	Not applicable	Not applicable	1.0	Recommended NOEL for Florida DER (MacDonald 1993).
Chromium (hexavalent)	Not applicable	Not applicable	8.1	TRV is an ERL value for total chromium (Long et al. 1995).
Copper	Not applicable	Not applicable	28	Recommended NOEL for Florida DER (MacDonald 1993).
Total Cyanide	Not applicable	Not applicable	0. 1	TRV is a U.S. EPA Region V guideline value for classification of sediments for determining the suitability of dredged material for open water disposal, as cited in Hull and Suter II (1994).

TABLE E-4

MARINE/ESTUARINE SEDIMENT TOXICITY REFERENCE VALUES

(Page 6 of 8)

Compound	Marine/Estuarine Surface Water TRV[a]	K_{oc} Value[b]	Bed Sediment TRV (dry weight)	Reference and Notes [c]
Lead	Not applicable	Not applicable	21.0	Recommended NOEL for Florida DER (MacDonald 1993).
Mercuric chloride	Not applicable	Not applicable	0.1	No toxicity data available for divalent inorganic mercury. Total mercury is used as surrogate. Recommended NOEL for Florida DER (MacDonald 1993).
Methyl mercury	Not applicable	Not applicable	0.1	No toxicity data available for methyl mercury. Total mercury is used as surrogate. Recommended NOEL for Florida DER (MacDonald 1993).
Nickel	Not applicable	Not applicable	20.9	TRV is an ERL value (Long et al. 1995).
Selenium	Not applicable	Not applicable	Not Available	Screening or toxicity value not available.
Silver	Not applicable	Not applicable	0.5	Recommended NOEL for Florida DER (MacDonald 1993).
Thallium	Not appliable	Not applicable	Not available	Screening or toxicity value not available.
Zinc	Not applicable	Not applicable	68	Recommended NOEL for Florida DER (MacDonald 1993).

TABLE E-4

MARINE/ESTUARINE SEDIMENT TOXICITY REFERENCE VALUES

(Page 7 of 8)

Notes:

a Sediment TRVs are in units of micrograms per kilogram (μg/kg) and milligrams per kilograms (mg/kg) for organic and inorganic constituents, respectively.

b Values are in units of liters per kilogram (L/kg). K_{oc} = Organic carbon normalized sorption coefficient. References and equations used to calculate values are provided in Appendix A.

c The references refer to the study or studies from which the endpoint and concentrations were identified. Complete reference citations are provided below.

d Sediment TRV calculated with the following equation:

Sediment TRV = Marine/estuarine surface water TRV (Table E-2) * K_{oc} * $f_{oc,bs}$

where,

K_{oc} = organic carbon partition coefficient, and
$f_{oc,bs}$= fraction of organic carbon in bed sediment, assumed to be 1 percent = 0.01.

K_{oc} values are discussed in Appendix A.

EqP = Equilibrium Partitioning
ERL = Effects Range-Low
HMW = High molecular weight
LEL = Lowest Effect Level
NOEL = No Observed Effect Level
TRV = Toxicity Reference Value

TABLE E-4

MARINE/ESTUARINE SEDIMENT TOXICITY REFERENCE VALUES

(Page 8 of 8)

REFERENCES

Default TRVs for sediments in marine and estuarine habitats were identified from several sets of toxicity values (standards, benchmarks, and guidelines) presented below. While some compound-specific marine/estuarine sediment toxicity information is available in the scientific literature, available toxicity values were not used because of the compexity in understanding the role of naturally-occurring sediment features (such as grain size, ammonia, sulfide, soil type, and organic carbon content) in toxicity to benthic invertebrates. Among these sets of value, the lowest available toxicity value for a particular compound was adopted as the TRV. In many cases, a default TRV was calculated from the corresponding freshwater TRV using EPA's equilibrium partitioning approach, assuming a 4 percent organic carbon content.

Hull, R.N. and G.W. Suter II. 1994. *Toxicological Benchmarks for Screening Contaminants of Potential Concern for Effects on Sediment-Associated Biota: 1994 Revision.* ES/ER/TM-95/R1. Environmental Sciences Division, Oak Ridge National Laboratory. Oak Ridge, Tennessee. June.

Long, E.R., and L.G. Morgan. 1991. *The Potential for Biological Effects of Sediment-Sorbed Contaminants Tested in the National Status and Trends Program.* National Oceanic and Atmospheric Administration (NOAA) Technical Memorandum No. 5, OMA52, NOAA National Ocean Service. August.

Long, E.R., D.D. MacDonald, S.L. Smith, and F.D. Calder. 1995. "Incidence of Adverse Biological Effects Within Ranges of Chemical Concentrations in Marine and Estuarine Sediments." *Environmental Management*. Volume 19. Pages 81-97.

MacDonald, D.D. 1993. *Development of an Approach to the Assessment of Sediment Quality in Florida Coastal Waters*. Florida Department of Environmental Regulation. Tallahassee, Florida. January.

Persaud, D., R. Jaaguagi, and A. Hayton. 1993. *Guidelines for the Protection and Management of Aquatic Sediment Quality in Ontario*. Ontario Ministry of the Environment. Queen's Printer of Ontario. March.

U.S. EPA. 1993. *Technical Basis for Deriving Sediment Quality Criteria for Nonionic Organic Contaminants for the Protection of Benthic Organisms by Using Equilibrium Partitioning*. Office of Water. EPA-822-R-93-011. September.

Washington State Department of Ecology. 1991. *Sediment Management Standards*. Washington Administrative Code 173-204.

TABLE E-5

TERRESTRIAL PLANT TOXICITY REFERENCE VALUES

(Page 1 of 15)

Compound	Basis for TRV				TRV [c]	Reference and Notes [d]
	Duration and Endpoint [a]	Test Organism	Concentration	Uncertainty Factor [b]		
Polychlorinateddibenzo-p-dioxins (μg/kg)						
2,3,7,8-TCDD	--	--	--	--	--	Toxicity value not identified.
Polynuclear aromatic hydrocarbons (PAH) (μg/kg)						
Total high molecular weight (HMW) PAH	Chronic NOAEL	Wheat	1,200	Not applicable	1,200	Benzo(a)pyrene toxicity used as representative toxicity of all HMW PAHs. This TRV may be used to characterize risk of total HMW PAHs to terrestrial plants.
Benzo(a)pyrene	Chronic NOAEL	Wheat	1,200	Not applicable	1,200	Sims and Overcash (1983)
Benzo(a)anthracene	Not available	--	--	--	1,200	Toxicity value not available. Benzo(a)pyrene used as surrogate.
Benzo(b)fluoranthene	Chronic NOAEL	Wheat	1,200	Not applicable	1,200	Sims and Overcash (1983).
Benzo(k)fluoranthene	Not available	--	--	--	1,200	Toxicity value not available. Benzo(a)pyrene used as surrogate.
Chrysene	Not available	--	--	--	1,200	Toxicity value not available. Benzo(a)pyrene used as surrogate.
Dibenz(a,h)anthracene	Not available	--	--	--	1,200	Toxicity value not available. Benzo(a)pyrene used as surrogate.

TABLE E-5

TERRESTRIAL PLANT TOXICITY REFERENCE VALUES

(Page 2 of 15)

Compound	Basis for TRV				TRV [c]	Reference and Notes [d]
	Duration and Endpoint [a]	Test Organism	Concentration	Uncertainty Factor [b]		
Indeno(1,2,3-cd)pyrene	Not available	--	--	--	1,200	Toxicity value not available. Benzo(a)pyrene used as surrogate.
Polychlorinated biphenyls (PCB) (μg/kg)						
Aroclor 1016	--	--	--	--	10,000	No toxicity value available. Aroclor 1254 TRV adopted as surrogate.
Aroclor 1254	Chronic NOAEL	Soybean shoot weight	10,000	Not applicable	10,000	Value for toxicity of Aroclor 1254 (Weber and Mrozek 1979).
Nitroaromatics (μg/kg)						
1,3-Dinitrobenzene	--	--	--	--	--	Toxicity value not available.
2,4-Dinitrotoluene	--	--	--	--	--	Toxicity value not available.
2,6-Dinitrotoluene	--	--	--	--	--	Toxicity value not available.
Nitrobenzene	--	--	--	--	--	Toxicity value not available.
Pentachloronitrobenzene	--	--	--	--	--	Toxicity value not available.
Phthalate esters (μg/kg)						
Bis(2-ethylhexyl)phthalate	--	--	--	--	--	Toxicity value not available.
Di(n)octyl phthalate	--	--	--	--	--	Toxicity value not available.
Volatile organic compounds (μg/kg)						

TABLE E-5

TERRESTRIAL PLANT TOXICITY REFERENCE VALUES

(Page 3 of 15)

Compound	Basis for TRV				TRV [c]	Reference and Notes [d]
	Duration and Endpoint [a]	Test Organism	Concentration	Uncertainty Factor [b]		
Acetone	--	--	--	--	--	Toxicity value not available.
Acrylonitrile	--	--	--	--	--	Toxicity value not available.
Chloroform	--	--	--	--	--	Toxicity value not available.
Crotonaldehyde	--	--	--	--	--	Toxicity value not available.
1,4-Dioxane	--	--	--	--	--	Toxicity value not available.
Formaldehyde	--	--	--	--	--	Toxicity value not available.
Vinyl chloride	--	--	--	--	--	Toxicity value not available.
Other chlorinated organics (µg/kg)						
Hexachlorobenzene	--	--	--	--	--	Toxicity value not available.
Hexachlorobutadiene	--	--	--	--	--	Toxicity value not available.
Hexachlorocyclopentadiene	Acute EC50	Lettuce growth	10,000	0.01	100	Hulzebos et al. (1993)
Pentachlorobenzene	--	--	--	--	--	Toxicity value not available.
Pentachlorophenol	Chronic LOAEL	Rice	17,300	0.1	1,730	Nagasawa et al. (1981)
Pesticides (µg/kg)						
4,4'-DDE	--	--	--	--	--	Toxicity value not available.

TABLE E-5

TERRESTRIAL PLANT TOXICITY REFERENCE VALUES

(Page 4 of 15)

Compound	Basis for TRV				TRV [c]	Reference and Notes [d]
	Duration and Endpoint [a]	Test Organism	Concentration	Uncertainty Factor [b]		
Heptachlor	Chronic NOAEL	Carrot	1,000	Not applicable	1,000	Ahrens and Kring (1968)
Hexachlorophene	--	--	--	--	--	Toxicity value not available.
Inorganics (mg/kg)						
Aluminum	Subchronic NOAEL	White clover seedling establishment	50	0.1[e]	5	Mackay et al. (1990)
Antimony	Not specified	Not specified	5	0.1[e]	0.5	Kabata-Pendias and Pendias (1992)
Arsenic	Chronic LOAEL	Corn yield (weight)	10	0.1	1	Woolson et al. (1971)
Barium	Chronic LOAEL	Barley shoot growth	500	0.01[e]	5	Chaudry et al. (1977)
Beryllium	Not specified	Not specified	10	0.01[e]	0.1	Kabata-Pendias and Pendias (1992)
Cadmium	Chronic LOAEL	Spruce seedling growth	2	0.1[e]	0.2	Burton et al. (1984)
Chromium (hexavalent)	Subchronic EC50	Lettuce growth	1.8	0.01	0.018	Adema and Hazen (1989)
Copper	Chronic LOAEL	Barley	10	0.1	1.0	Toivonem and Hofstra (1979)

TABLE E-5

TERRESTRIAL PLANT TOXICITY REFERENCE VALUES

(Page 5 of 15)

Compound	Basis for TRV				TRV [c]	Reference and Notes [d]
	Duration and Endpoint [a]	Test Organism	Concentration	Uncertainty Factor [b]		
Cyanide, total	--	--	--	--	--	Toxicity value not available.
Lead	Chronic LOAEL	Senna	46	0.1	4.6	Krishnayya and Bedi (1986)
Mercuric chloride	Acute NOEC	Barley	34.9	0.01[e]	0.349	Panda et al. (1992)
Methyl mercury	--	--	--	--	--	Toxicity value not available.
Nickel	Chronic NOAEL	Bush bean shoot growth	25	Not applicable	25	Wallace et al. (1977)
Selenium	Subchronic NOAEL	Alfalfa shoot weight	0.5	0.1	0.05	Wan et al. (1988)
Silver	Not specified	Not specified	2	0.01[e]	0.02	Kabata-Pendias and Pendias (1992)
Thallium	Not specified	Not specified	1	0.01[e]	0.01	Kabata-Pendias and Pendias (1992)
Zinc	Chronic LOAEL	Spring barley	9	0.1	0.9	Davis, Beckett, and Wollan (1978)

TABLE E-5

TERRESTRIAL PLANT TOXICITY REFERENCE VALUES

(Page 6 of 15)

Notes:

a To evaluate exposure duration, the following general guidelines were used: Chronic duration represents exposures occurring about 10 or more days, including exposure during a critical life stage, such as germination and shoot development. Subchronic duration generally lasts 2 days through several days, however a sensitive life stage is not exposed. Acute duration generally includes exposures occurring 0 to 2 days.

b Uncertainty factors are used to extrapolate a toxicity value to a chronic NOAEL TRV. See Chapter 5 (Section 5.4) of the SLERAP for a discussion on the use of uncertainty factors.

c TRV was calculated by multiplying the toxicity value with the uncertainty factor.

d The references refer to the source of the toxicity value. Complete reference citations are provided below.

e Best scientific judgment was used to identify uncertainty factor. See Chapter 5 (Section 5.4.1.2) for a discussion on the use of best scientific judgement. Factors evaluated include test duration, ecological relevance of endpoint, and experimental design.

EC50 = Effective concentration for 50 percent of the test organisms.
HWC = High molecular weight
LOAEL = Lowest Observed Adverse Effects Level
NOAEL = No Observed Adverse Effects Level
NOEC = No Observed Effects Concentration
TRV = Toxicity Reference Value

TABLE E-5

TERRESTRIAL PLANT TOXICITY REFERENCE VALUES

(Page 7 of 15)

REFERENCES

Efroymson, Will, Suter II, and Wooten (1997) provides a comprehensive review of ecologically-relevant terrestrial plant toxicity information. This source was reviewed to identify studies to develop TRVs for terrestrial plant. Based on the information presented, one or more references were obtained and reviewed to identify compound-specific toxicity values. For some compounds, the available information identified a single study meeting the requirements for a TRV, as discussed in Chapter 5 (Section 5.4) of the SLERAP. In most cases, each reference was obtained and reviewed to identify a single toxicity value to develop a TRV for each compound. In a few cases where a primary study could not be obtained, a toxicity value is based on a secondary source. As noted below, additional compendia were reviewed to identify toxicity studies to review. For compounds not discussed in Efroymson, Will, Suter II, and Wooten (1997), the scientific literature was searched, and relevant studies were obtained and reviewed. The references reviewed are listed below. The study selected for the TRV is highlighted in bold.

Benzo(a)pyrene

Sims R.C. and Overcash M.R. 1983. "Fate of Polynuclear Aromatic Compounds (PNAs) in Soil-Plant Systems." *Residue Reviews*. Volume 88.

Benzo(k)fluoranthene

Sims R.C. and Overcash M.R. 1983. "Fate of Polynuclear Aromatic Compounds (PNAs) in Soil-Plant Systems." *Residue Reviews*. Volume 88.

Aroclor 1254

Weber, J.B., and E. Mrozek, Jr. 1979. "Polychlorinated Biphenyls: Phytotoxicity, Absorption, and Translocation by Plants, and Inactivation by Activated Carbon." *Bulletin of Environmental Contamination and Toxicology*. Volume 23. Pages 412-417. As cited in Will and Suter II (1995b).

Weber, J. B. and E. Mrozek, Jr. 1979. "Polychlorinated Biphenyls: Phytotoxicity, Absorption and Translocation by Plants, and Inactivation by Activated Carbon". *Bulletin of Environmental Contamination and Toxicology*. Volume 23. Pages 412-17.

Nitroaromatics

McFarlane, C. M., T. Pfleeger, and J. Fletcher. 1990. "Effect, Uptake and Disposition of Nitrobenzene in Several Terrestrial Plants." *Environmental Toxicology and Chemistry*. Volume 9. Pages 513-520.

TABLE E-5

TERRESTRIAL PLANT TOXICITY REFERENCE VALUES

(Page 8 of 15)

Hexachlorocyclopentadiene

Hulzebos, E.M., D.M.M. Adema, E.M. Dirven-van Breeman, L. Henzen, W.A. van Dis, H.A. Herbold, J.A. Hoekstra, R. Baerselman, and C.A.M. van Gestel. 1993. "Phototoxicity Studies with *Latuca sativa* in soil and soil nutrient solution." *Environmental Toxicology and Chemistry*. Volume 12. Pages 1079-1094.

Pentachlorophenol

Nagasawa, S., and others. 1981. "Concentration of PCP Inhibiting the Development of Roots at the Early Growth Stage of Rice and the Difference of Susceptibilities in Varieties." *Bull. Fac. Agricul*. Shimane Univ. Volume 15. Pages 101-108. As cited in U.S. Fish and Wildlife Service. 1989. *Pentachlorophenol Hazards to Fish, Wildlife, and Invertebrates: A Synoptic Review*. April.

van Gestel, C. A. M., D. M. M. Adema, and E. M. Dirven-van Breemen. 1996. "Phytotoxicity of Some Chloroanilines and Chlorophenols, in Relation to Bioavailability in Soil." *Water, Air and Soil Pollution.* Volume 88. Pages 119-132.

Heptachlor

Ahrens, J.F., and J.B. Kring. 1968. "Reduction of Residues of Heptachlor and Chlordane in Carrots with Soil Applications of Activated Carbon." *Journal of Economic Entomology*. Volume 61. Pages 1540-1543.

Aluminum

Mackay, A.D., J.R. Caradus, and M.W. Pritchard. 1990. "Variation for Aluminum Tolerance in White Clover." *Plant and Soil*. Volume 123. Pages 101-105.

Godbold, D. L., and C. Kettner. 1991. "Use of Root Elongation Studies to Determine Aluminum and Lead Toxicity in *Picea abies* Seedlings." *Journal Plant Physiology*. Volume 138. Pages 231-235.

Görransson, A. and T. D. Eldhuset. 1991." Effects of Aluminum on Growth and Nutrient Uptake of Small *Picea abies* and *Pinus sylvestris* Plants." *Trees.* Volume 5. Page 136-42.

Llugany, M., C. Poschenrieder, and J. Barcelo. 1995. "Monitoring of Aluminum-Induced Inhibition of Root Elongation in Four Maize Cultivars Differing in Tolerance to Aluminum and Proton Toxicity." *Physiologia Plantarum.* Volume 93. Pages 265-271.

Wheeler, D. M. and J. M. Follet. 1991. "Effect of Aluminum on Onions, Asparagus and Squash." *Journal Plant Nutrients.* Volume 14(9). Page 897-912.

TABLE E-5

TERRESTRIAL PLANT TOXICITY REFERENCE VALUES

(Page 9 of 15)

Antimony

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TABLE E-6

SOIL INVERTEBRATE TOXICITY REFERENCE VALUES

(Page 1 of 12)

Compound	TRV				TRV [c]	Reference and Notes [d]
	Duration and Endpoint [a]	Test Species	Concentration	Uncertainty Factor [b]		
Polychlorinateddibenzo-p-dioxins (μg/kg)						
2,3,7,8-TCDD	Chronic (85-day); no mortality reported at 5,000 μg/kg	Earthworm (*Allolobophora caliginosa*)	5,000	0.1[e]	500	Toxicity value for 2,3,7,8-TCDD (Reinecke and Nash 1984). UF applied to concentration because mortality only endpoint available and data not subjected to statistical analysis.
Polynuclear aromatic hydrocarbons (PAH) (μg/kg)						
Total HMW PAH	Not available	--	--	--	25,000	Benzo(a) pyrene used as surrogate for HMW PAH compounds.
Benzo(a)pyrene	Chronic (28-day) NOAEL for growth	Woodlouse (*Porcellio scaber*)	25,000	Not applicable	25,000	van Straalen and Verweij (1991)
Benzo(a)anthracene	Not available	--	--	--	25,000	Toxicity value not available. TRV for benzo(a)pyrene used as surrogate.
Benzo(b)fluoranthene	Not available	--	--	--	25,000	Toxicity value not available. TRV for benzo(a)pyrene used as surrogate.
Benzo(k)fluoranthene	Not available	--	--	--	25,000	Toxicity value not available. TRV for benzo(a)pyrene used as surrogate.
Chrysene	Not available	--	--	--	25,000	Toxicity value not available. TRV for benzo(a)pyrene used as surrogate.
Dibenz(a,h)anthracene	Not available	--	--	--	25,000	Toxicity value not available. TRV for benzo(a)pyrene used as surrogate.
Indeno(1,2,3-cd)pyrene	Not available	--	--	--	25,000	Toxicity value not available. TRV for benzo(a)pyrene used as surrogate.

TABLE E-6

SOIL INVERTEBRATE TOXICITY REFERENCE VALUES

(Page 2 of 12)

Compound	TRV				TRV [c]	Reference and Notes [d]
	Duration and Endpoint [a]	Test Species	Concentration	Uncertainty Factor [b]		
Polychlorinated biphenyls (PCB) (μg/kg)						
Aroclor 1016	Acute median LC50	Earthworm (*Eisenia foetida*)	251,000	0.01	2,510	Rhett et al. (1989).
Aroclor 1254	Acute median LC50	Earthworm (*Eisenia foetida*)	251,000	0.01	2,510	Rhett et al. (1989).
Nitroaromatics (μg/kg)						
1,3-Dinitrobenzene	--	--	--	--	2,260	Toxicity value not available. Nitrobenzene used as surrogate.
2,4-Dinitrotoluene	--	--	--	--	--	Toxicity value not available.
2,6-Dinitrotoluene	--	--	--	--	--	Toxicity value not available.
Nitrobenzene	Subchronic (14-day) LC50	Earthworm (species uncertain)	226,000	0.01[e]	2,260	Neuhauser et al. (1986).
Pentachloronitrobenzene	--	--	--	--		Toxicity value not available.
Phthalate esters (μg/kg)						
Bis(2-ethylhexyl)phthalate	--	--	--	--	--	Toxicity value not available.
Di(n)octyl phthalate	--	--	--	--	--	Toxicity value not available.
Volatile organic compounds (μg/kg)						
Acetone	--	--	--	--	--	Toxicity value not available.
Acrylonitrile	--	--	--	--	--	Toxicity value not available.

TABLE E-6

SOIL INVERTEBRATE TOXICITY REFERENCE VALUES

(Page 3 of 12)

Compound	TRV				TRV [c]	Reference and Notes [d]
	Duration and Endpoint [a]	Test Species	Concentration	Uncertainty Factor [b]		
Chloroform	--	--	--	--	--	Toxicity value not available.
Crotonaldehyde	--	--	--	--	--	Toxicity value not available.
1,4-Dioxane	--	--	--	--	--	Toxicity value not available.
Formaldehyde	--	--	--	--	--	Toxicity value not available.
Vinyl chloride	--	--	--	--	--	Toxicity value not available.
Other chlorinated organics (µg/kg)						
Hexachlorobenzene	--	--	--	--	--	Toxicity value not available.
Hexachlorobutadiene	--	--	--	--	--	Toxicity value not available.
Hexachlorocyclopentadiene	--	--	--	--	--	Toxicity value not available.
Pentachlorobenzene	LC50 of unspecified duration	Earthworm (species uncertain)	115,000	0.01[e]	1,150	van Gestel et al. (1991)
Pentachlorophenol	Chronic (21-day) NOAEL for hatching success	Earthworm (*Eisenia andrei*)	10,000	Not applicable	10,000	van Gestel et al. (1988)
Pesticides (µg/kg)						
4,4'-DDE	--	--	--	--	--	Toxicity value not available.
Heptachlor	--	--	--	--	--	Toxicity value not available.
Hexachlorophene	--	--	--	--	--	Toxicity value not available.
Inorganics (mg/kg)						

TABLE E-6

SOIL INVERTEBRATE TOXICITY REFERENCE VALUES

(Page 4 of 12)

Compound	TRV				TRV [c]	Reference and Notes [d]
	Duration and Endpoint [a]	Test Species	Concentration	Uncertainty Factor [b]		
Aluminum	--	--	--	--	--	Toxicity value not available.
Antimony	--	--	--	--	--	Toxicity value not available.
Arsenic	Chronic (56-day); reduced cocoon production reported at single concentration tested	Earthworm (*Eisenia fetida*)	25	0.01[e]	0.25	Fischer and Koszorus (1992)
Barium	--	--	--	--	--	Toxicity value not available.
Beryllium	--	--	--	--	--	Toxicity value not available.
Cadmium	Chronic (4-month) NOAEL for cocoon production	Earthworm (*Dendrobaena rubida*)	10	Not applicable	10	Bengtsson and et al. (1986)
Chromium (hexavalent)	Chronic (60-day); survival reduced 25 percent at lowest tested concentration	Earthworm (*Octochaetus pattoni*)	2	0.1[e]	0.2	Abbasi and Soni (1983)
Copper	Chronic (56-day) NOAEL for cocoon production	Earthworm (*Eisenia fetida*)	32.0	Not applicable	32.0	Spurgeon et al. (1994)
Cyanide, total	--	--	--	--	--	Toxicity value not available.
Lead	Chronic (4-month) NOAEL for cocoon production	Earthworm (*Dendrobaena rubida*)	100	Not applicable	100	Bengtsson et al. 1986

TABLE E-6

SOIL INVERTEBRATE TOXICITY REFERENCE VALUES

(Page 5 of 12)

Compound	TRV				TRV [c]	Reference and Notes [d]
	Duration and Endpoint [a]	Test Species	Concentration	Uncertainty Factor [b]		
Mercuric chloride	Not available	--	--	--	2.5	Toxicity value not available. TRV for methyl mercury used as a surrogate.
Methyl mercury	Chronic (12-week) NOAEL for segment regeneration and survival	Earthworm (*Eisenia foetida*)	2.5	Not applicable	2.5	Beyer et al. (1985). Wet weight NOAEL of 1 mg/kg converted to corresponding dry weight NOAEL based on 60 percent moisture content. Uncertainty factor of 0.1 used because segment regeneration may not be a sensitive endpoint.
Nickel	Chronic (20-week) NOAEL for cocoon production	Earthworm (*Eisenia foetida*)	100	Not applicable	100	Malecki et al. (1982)
Selenium	Chronic; reduced cocoon production at single tested concentration	Earthworm (*Eisenia foetida*)	77	0.1[e]	7.7	Fischer and Koszorus (1992)
Silver	--	--	--	--	--	Toxicity value not available.
Thallium	--	--	--	--	--	Toxicity value not available.
Zinc	Chronic (56-day) NOEC for cocoon production	Earthworm (*Eisenia fetida*)	199	Not applicable	199	Spurgeon et al. (1994)

TABLE E-6

SOIL INVERTEBRATE TOXICITY REFERENCE VALUES

(Page 6 of 12)

Notes:

a - duration, the following general guidelines were used: Chronic duration represents exposures occurring about 10 or more days, including exposure during a critical life stage encompassing a sensitive endpoint. Subchronic duration generally lasts 2 days through several days, however a sensitive life stage is not exposed. Acute duration generally includes exposures from 0 to 2 days.

b Uncertainty factors are used to extrapolate a toxicity value to a chronic NOAEL TRV. See Chapter 5 (Section 5.4) of the SLERAP for a discussion on the use of uncertainty factors.

c TRV was calculated by multiplying the toxicity value with the uncertainty factor.

d The references refer to the source of the toxicity value. Complete reference citations are provided below.

e Best scientific judgment used to identify uncertainty factor. See Chapter 5 (Section 5.4.1.2) for a discussion on the use of best scientific judgement. Factors evaluated include test duration, ecological relevance of measured effect, experimental design, and availability of toxicity data.

HMW	=	High molecular weight
LC50	=	Concentration lethal to 50 percent of the test organisms.
NOAEL	=	No Observed Adverse Effects Level
NOEC	=	No Observed Effects Level
UF	=	Uncertainty Factor
TRV	=	Toxicity Reference Value

TABLE E-6

SOIL INVERTEBRATE TOXICITY REFERENCE VALUES

(Page 7 of 12)

REFERENCES

Efroymson, Will, and Suter II (1997) provides a comprehensive review of ecologically-relevant soil invertebrate toxicity information. This source was reviewed to identify studies to develop TRVs for invertebrates. Effects of compounds on microbial communities were not considered. Based on the information presented, one or more references were obtained and reviewed to identify compound-specific toxicity values. For some compounds, the available information identified a single study meeting the requirements for a TRV, as discussed in Section 5.4. In most cases, each reference was obtained and reviewed to identify a single toxicity value to develop a TRV for each compound. In a few cases where a primary study could not be obtained, a toxicity value is based on a secondary source. As noted below, additional compendia were reviewed to identify toxicity studies to review. For compounds not discussed in Efroymson, Will, and Suter II (1997), the scientific literature was searched, and relevant studies were obtained and reviewed. The references reviewed are listed below. The study selected for the TRV is highlighted in bold.

Polychlorinated dibenzo(p)dioxins

Reinecke, A.J., and R.G. Nash. 1984. "Toxicity of 2,3,7,8-TCDD and Short-Term Bioaccumulation by Earthworms (Oligochaeta)." *Soil Biology* Biochemistry. Volume 16. Pages 45-49. As cited in U.S. Fish and Wildlife Service. 1986. *Dioxin Hazards to Fish, Wildlife, and Invertebrates: A Synoptic Review*. Biological Report 85 (1.8). May.

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van Brummelen, T.C., and S.C. Stuijfzand. 1993. "Effects of benzo(a)pyrene on survival, growth and energy reserves in terrestrial isopods *Oniscus asellus* and *Porcellio scaber*." *Science of the Total Environment. Supplement.* Pages 921-930.

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Polychlorinated biphenyls

Rhett, G., and others. 1989. "Rate and Effects of PCB Accumulation on *Eisenia foetida*." U.S. Army Corps of Engineers. Waterways Experiment Station. Vicksburg, Mississippi. September 21.

Nitrobenzene

TABLE E-6

SOIL INVERTEBRATE TOXICITY REFERENCE VALUES

(Page 8 of 12)

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TABLE E-6

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TABLE E-6

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TABLE E-7

MAMMAL TOXICITY REFERENCE VALUES

(Page 1 of 15)

Compound	Basis for Toxicity Reference Value (TRV)				TRV	Reference and Notes [d]
	Duration and Endpoint [a]	Test Organism	Dose [b]	Uncertainty Factor [c]		
Polychlorinateddibenzo-p-dioxins (μg/kg BW-day)						
2,3,7,8-TCDD	Chronic (multigenerational) NOAEL for reproduction	Rat	0.001	Not applicable	0.001	Murray et al. (1979). TRV based on toxicity of 2,3,7,8-TCDD.
Polynuclear aromatic hydrocarbons (PAH) (μg/kg BW-day)						
Total high molecular weight (HMW) PAH	--	--	--	--	100	TRV based on benzo(a)pyrene toxicity. This TRV should be assessing the risk of Total HMW PAH.
Benzo(a)pyrene	Acute (10 days) LOAEL (reproductive effects)	Mouse	10,000	0.01	100	Mackenzie and Angevine (1981)
Benzo(a)anthracene	Single dose LOAEL (gastrointestinal effects)	Mouse	16,666	0.01	167	Bock and King (1959)
Benzo(b)fluoranthene	--	--	--	--	--	Toxicity value not available.
Benzo(k)fluoranthene	--	--	--	--	--	Toxicity value not available.
Chrysene	--	--	--	--	--	Toxicity value not available.
Dibenz(a,h)anthracene	Subchronic (15 days) LOAEL (reduced growth rate)	Rat	200	0.01[e]	2	Haddow et al. (1937)
Indeno(1,2,3-cd)pyrene	--	--	--	--	--	Toxicity value not available.

TABLE E-7

MAMMAL TOXICITY REFERENCE VALUES

(Page 2 of 15)

Compound	Basis for Toxicity Reference Value (TRV)				TRV	Reference and Notes [d]
	Duration and Endpoint [a]	Test Organism	Dose [b]	Uncertainty Factor [c]		
Polychlorinated biphenyls (PCB) (μg/kg BW-day)						
Aroclor 1016	Subchronic (14.5 weeks) LOAEL (mortality)	Mink	20.6	0.01	0.206	Aulerich et al. (1985). TRV based on toxicity of 3,4,5-hexachlorobiphenyl.
Aroclor 1254	Subchronic (14.5 weeks) LOAEL (mortality)	Mink	20.6	0.01	0.206	Aulerich et al. (1985). TRV based on toxicity of 3,4,5-hexachlorobiphenyl.
Nitroaromatics (μg/kg BW-day)						
1,3-Dinitrobenzene	Chronic (16 weeks) NOAEL	Rat	1,051	1.0	1,051	Cody et al. (1981)
2,4-Dinitrotoluene	Chronic (24 months) NOAEL	Dog	700	1.0	700	Ellis et al. (1979)
2,6-Dinitrotoluene	Single dose LOAEL (mortality)	Dog	4,000	0.01	400	Lee et al. (1976)
Nitrobenzene	--	--	--	--	--	Toxicity value not available.
Pentachloronitrobenzene	Chronic (2 years) NOAEL	Mouse	458,333	1.0	458,333	National Toxicology Program (1987)
Phthalate esters (μg/kg BW-day)						
Bis(2-ethylhexyl)phthalate	Chronic (2 years) NOAEL	Rat	60,000	1.0	60,000	Carpenter et al. (1953)
Di(n)octyl phthalate	Chronic (105 days) NOAEL	Mouse	7,500,000	1.0	7,500,000	Heindel et al. (1989)
Volatile organic compounds (μg/kg BW-day)						
Acetone	Subchronic (90 days) NOAEL	Albino Rat, male	100,000	0.1	10,000	U.S. EPA (1986)
Acrylonitrile	Chronic (2 years) LOAEL (lesions and other organ effects)	Rat	4,600	0.1	460	Quast et al. (1980)
Chloroform	Chronic (80 weeks) NOAEL	Mouse	60,000	1.0	60,000	Roe et al. (1979)

TABLE E-7

MAMMAL TOXICITY REFERENCE VALUES

(Page 3 of 15)

Compound	Basis for Toxicity Reference Value (TRV)				TRV	Reference and Notes [d]
	Duration and Endpoint [a]	Test Organism	Dose [b]	Uncertainty Factor [c]		
Crotonaldehyde	Acute (4-hour) LD50	Rat	8,000	0.01	80	Rinehart (1967)
1,4-Dioxane	Chronic (23 months) LOAEL (lung tumors)	Guinea Pig	1,069,767	0.1	106,777	Hoch-Ligeti and Argus (1970)
Formaldehyde	Acute (single dose) LOAEL (mortality)	Rat	230,000	0.01	2,300	Tsuchiya et al. (1975)
Vinyl chloride	Chronic (2 years) NOAEL	Rat	1,700	0.1	170	Feron et al. (1981)
Other chlorinated organics (μg/kg BW-day)						
Hexachlorobenzene	Chronic (>247 days) NOAEL	Rat	1,600	1.0	1,600	Grant et al. (1977)
Hexachlorobutadiene	Chronic (2 years) NOAEL	Rat	200	1.0	200	Kociba et al. (1977)
Hexachlorocyclopentadiene	Subchronic (13 weeks) NOAEL	Rat	38,000	0.1	3,800	Abdo et al. (1984)
Pentachlorobenzene	Chronic (180 days) NOAEL	Rat	7,250	1.0	7,250	Linder et al. (1980)
Pentachlorophenol	Subchronic (62 days) NOAEL	Rat	3,000	0.1	300	Schwetz et al. (1978)
Pesticides (μg/kg BW-day)						
4,4'-DDE	Subchronic (5 weeks) NOAEL	Rat	10,000	0.1	1,000	Kornburst et al. (1986)
Heptachlor	Subchronic (60 days) LOAEL (mortality)	Rat	250	0.01	2.5	Green (1970)
Hexachlorophene	Acute LD50	Rat	560,000	0.01	5600	Meister (1994)
Inorganics (mg/kg BW-day)						
Aluminum	Chronic (>1 year) LOAEL (growth)	Rat	19.3	0.1	1.93	Ondreicka et al. (1966)

TABLE E-7

MAMMAL TOXICITY REFERENCE VALUES

(Page 4 of 15)

Compound	Basis for Toxicity Reference Value (TRV)				TRV	Reference and Notes [d]
	Duration and Endpoint [a]	Test Organism	Dose [b]	Uncertainty Factor [c]		
Antimony	Chronic (4 years) LOAEL (mortality)	Rat	0.66	0.1	0.066	Schroeder et al. (1970)
Arsenic	Chronic (2 years) NOAEL	Dog	1.25	1.0	1.25	Byron et al. (1967)
Barium	Chronic (16 months) NOAEL	Rat	0.51	1.0	0.51	Perry et al. (1983)
Beryllium	Chronic (>1 year) NOAEL	Rat	0.66	1.0	0.66	Schroeder and Mitchner (1975)
Cadmium	Chronic (>150 days) LOAEL (reproduction)	Mouse	2.52	0.01	0.0252	Schroeder and Mitchner (1971)
Chromium (hexavalent)	Chronic (1 year) NOAEL	Rat	3.5	1.0	3.5	MacKenzie et al. (1958)
Copper	Chronic (357 days) NOAEL	Mink	12.0	1.0	12.0	Aulerich et al. (1982)
Total Cyanide	Chronic (2 years) NOAEL	Rat	24	1.0	24	Howard and Hanzal (1955)
Lead	Chronic (>150 days) LOAEL (mortality)	Mouse	3.75	0.01	0.0375	Schroeder and Mitchner (1971)
Mercuric chloride	Chronic (6 months) NOAEL (reproduction)	Mink	1.01	1.0	1.01	Aulerich et al. (1974)
Methyl mercury	Subchronic (93 days) NOAEL	Rat	0.032	1.0	0.032	Verschuuren et al. (1976)
Nickel	Chronic (2 years) NOAEL	Rat	50	1.0	50	Ambrose et al. (1976)
Selenium	Chronic (>150 days) LOAEL (mortality)	Mouse	0.76	0.1	0.076	Schroeder and Mitchner (1971)
Silver	Chronic (125 days) LOAEL (hypoactivity)	Mouse	3.75	0.1	0.375	Rungby and Danscher (1984)

TABLE E-7

MAMMAL TOXICITY REFERENCE VALUES

(Page 5 of 15)

Compound	Basis for Toxicity Reference Value (TRV)				TRV	Reference and Notes [d]
	Duration and Endpoint [a]	Test Organism	Dose [b]	Uncertainty Factor [c]		
Thallium	Subchronic (60 days) LOAEL (testicular function)	Rat	1.31	0.01[h]	0.0131	Formigli et al. (1986)
Zinc	Subchronic (13 weeks) NOAEL	Mouse	104	0.1	10.4	Maita et al. (1981)

Notes:

a The duration of exposure is defined as chronic if it represents about 10 percent or more of the test animal's lifetime expectancy. Acute exposures represent single exposure or multiple exposures occurring within about two weeks or less. Subchronic exposures are defined as multiple exposures occurring for less than 10 percent of the test animal's lifetime expectancy but more that 2 weeks.

b Reported values, which were dose in food or diet, were converted to dose based on body weight and intake rate using Opresko, Sample, and Suter 1996.

c Uncertainty factors are used to extrapolate a toxicity value to a chronic NOAEL TRV. See Chapter 5 (Section 5.4) for a discussion on the use of uncertainty factors. The TRV was calculated by multiplying the toxicity value by the uncertainty factor.

d The references refer to the study or studies from which the endpoint and doses were identified. Complete reference citations are provided at the end of this table.

e Best scientific judgement used to identify uncertainty factor. See Chapter 5 (Section 5.4.1.2) for a discussion of the use of best scientific judgement. Factors evaluated include test duration, ecological relevance of endpoint, experimental design, and availability of toxicity data.

HMW = High molecular weight
LD50 = Lethal dose to 50 percent of the test organisms.
LOAEL = Lowest Observed Adverse Effect Level
NOAEL = No Observed Adverse Effect Level
TRV = Toxicity Reference Value

TABLE E-7

MAMMAL TOXICITY REFERENCE VALUES

(Page 6 of 15)

REFERENCES

Sample, Opresko, and Suter II (1996) provides a comprehensive review of ecologically-relevant mammal toxicity information. This source was reviewed to identify studies to develop TRVs for mammals. Based on the information presented, one or more references were obtained and reviewed to identify compound-specific toxicity values. For some compounds, the available information identified a single study meeting the requirements for a TRV, as discussed in Section 5.4. In most cases, each reference was obtained and reviewed to identify a single toxicity value to develop a TRV for each compound. In a few cases where a primary study could not be obtained, a toxicity value is based on a secondary source. As noted below, additional compendia were reviewed to identify toxicity studies to review. For compounds not discussed in Sample, Opresko, and Suter II (1996), the scientific literature was searched, and relevant studies were obtained and reviewed. The references reviewed are listed below. The study selected for the TRV is highlighted in bold.

Polychlorinated dibenzo(p)dioxins

Murray, F.J., F.A. Smith, K.D. Nitschke, C.G. Humiston, R.J. Kociba, and B.A.Schwetz. 1979. "Three-Generation Reproduction Study of Rats Given 2,3,7,8-Tetrachlorodibenzo-p-dioxin (TCDD) in the Diet." *Toxicology and Applied Pharmacology*. Volume 50. Pages 241-252.

U.S. EPA. 1993. *Interim Report on Data and Methods for Assessment of 2,3,7,8-Tetrachlorodibenzop-dioxin Risks to Aquatic Life and Associated Wildlife.* EPA/600/R-93/055. Office of Research and Development. Washington, D.C. March. This report identified the four studies listed below.

Aulerich, R.J., R.K. Ringer, and S. Iwamoto. 1973. "Reproductive Failure and Mortality in Mink Fed on Great Lakes Fish." *Journal of Reproduction and Fertility*. Volume 19. Pages 365-376.

Aulerich, R.J., S.J. Bursian, and A.C. Napolitano. 1988. "Biological Effects of Epidermal Growth Factor and 2,3,7,8-Tetrachlorodibenzo-p-dioxin on Developmental Parameters of Neonatal Mink." *Archives of Environmental Contamination and Toxicology*. Volume 17. Pages 27-31.

Aulerich, R.J., S.J. Bursian, W.J. Breslin, B.A. Olson, and R.K. Ringer. 1985. "Toxicological Manifestations of 2,4,5,2',4',5'-, 2,3,6,2',3',6'-, and 3,4,5,3',4',5'-Hexachlorobiphenyl and Aroclor 1254 in Mink." Journal of Toxicology and Environmental Health. Volume 15. Pages 63-79.

Hochstein, J.R., R.J. Aulerich, and S.J. Bursain. 1988. "Acute Toxicity of 2,3,7,8-Tetrachlorodibenzo-p-dioxin to Mink." *Archives of Environmental Contamination and Toxicology*. Volume 17. Pages 33-37.

Benzo(a)pyrene

MacKenzie, K.M., and D.M. Angevine. 1981. "Infertility in Mice Exposed in Utero to Benzo(a)pyrene." *Biology of Reproduction*. Volume 24. Pages 183-191.

TABLE E-7

MAMMAL TOXICITY REFERENCE VALUES

(Page 7 of 15)

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Bock, F.G. and D.W. King. 1959. "A Study of the Sensitivity of the Mouse Forestomach Toward Certain Polycyclic Hydrocarbons." *Journal of the National Cancer Institute.* Volume 23. Page 833-839.

Dibenz(a,h)anthracene

Haddow, A., C.M. Scott, and J.D. Scott. 1937. "The Influence of Certain Carcinogenic and Other Hydrocarbons on Body Growth in the Rat." *Proceeding R. Soc. London. Series B.* Volume 122. Pages 477-507. As cited in IARC Monographs, 1983.

Polychlorinated biphenyls

Aulerich, R.J., S.J. Bursian, W.J. Breslin, B.A. Olson, and R.K. Ringer. 1985. "Toxicological Manifestations of 2,4,5-, 2',4',5'-, 2,3,6-, 2',3',6'- and 3,4,5-, 3',4',5'- Hexachlorobiphenyl and Aroclor 1254 in Mink." *Journal of Toxicology and Environmental Health.* Volume 15. Pages 63-79.

Aulerich, R. J. and R. K. Ringer. 1977. "Current Status of PCB Toxicity, Including Reproduction in Mink."*Archives of Environmental Containation and Toxicology*. Volume 6. Page 279.

ATSDR (Agency for Toxic Substances and Disease Registry). 1989. *Toxicological profile for Selected PCBs (Aroclor-1260, -1254, -1248, -1242, -1232, -1221, and -1016)*. ATSDR/TP-88/21.

Barsotti, D. A., R. J. Marlar and J. R. Allen. 1976. "Reproductive Dysfunction in Rhesus Monkeys Exposed to Low Llevels of Polychlorinated Biphenyls (Aroclor 1248)." *Food and Cosmetics Toxicology*. Volume 14. Pages 99-103.

Bleavins, M. R., R. J. Aulerich, and R. K. Ringer. 1980. "Polychlorinated Biphenyls (Aroclors 1016 and 1242): Effect on Survival and Reproduction in Mink and Ferrets." *Archives of Environmental Contamination and Toxicology* Volume 9. Pages 627-635.

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TABLE E-7

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TABLE E-8

BIRD TOXICITY REFERENCE VALUES

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Compound	Basis for TRV				TRV	Reference and Notes [d]
	Duration and Endpoint [a]	Test Organism	Dose[b]	Uncertainty Factor [c]		
Polychlorinateddibenzo(p)dioxins (μg/kg BW-day)						
2,3,7,8-TCDD	Subchronic (10 weeks) NOAEL	Ring-necked pheasant hen	0.01	Not applicable	0.01	Nosek et al. (1992). TRV based on toxicity of 2,3,7,8-TCDD.
Polynuclear aromatic hydrocarbons (PAH) (μg/kg BW-day)						
Total high molecular weight (HMW) PAH	--	--	--	--	0.14	TRV based on toxicity of benzo(k)fluoranthene. If TRVs are not available for all individual HMW PAHs, this TRV should be used to assess potential risk of Total HMW PAH.
Benzo(a)pyrene	Acute NOAEL	Chicken embryo	100	0.01	1.0	Brunström et al. (1991).
Benzo(a)anthracene	Acute LD50	Chicken embryo	79	0.01	0.79	Brunström et al. (1991).
Benzo(b)fluoranthene	--	--	--	--	0.14	No toxicity data available for benzo(b) fluoranthene. Benzo(k)fluoranthene used as surrogate.
Benzo(k)fluoranthene	Acute LD50	Chicken embryo	14	0.01	0.14	Brunström et al. (1991).
Chrysene	Acute LOAEL	Chicken embryo	100	0.01	1.0	Brunström et al. (1991).
Dibenz(a,h)anthracene	Acute LD50	Chicken embryo	39	0.01	0.39	Brunström et al. (1991).

TABLE E-8

BIRD TOXICITY REFERENCE VALUES

(Page 2 of 13)

Compound	Basis for TRV				TRV	Reference and Notes [d]
	Duration and Endpoint [a]	Test Organism	Dose[b]	Uncertainty Factor [c]		
Indeno(1,2,3-cd)pyrene	Acute LOAEL	Chicken embryo	100	0.01	1.0	Brunström et al. (1991).
Polychlorinated biphenyls (PCB) (μg/kg BW-day)						
Aroclor 1016	--	--	--	--	--	No toxicity data available. Aroclor 1254 TRV used as surrogate.
Aroclor 1254	Chronic (3 months) LOAEL (embryonic mortality)	Ring dove	720	0.1	72	Peakall et al. (1972). TRV based on toxicity of Aroclor 1254.
Nitroaromatics (μg/kg BW-day)						
1,3-Dinitrobenzene	Acute LD50	Redwing blackbird	42.2	0.01	0.422	Schafer (1972)
2,4-Dinitrotoluene	--	--	--	--	--	Toxicity value not available.
2,6-Dinitrotoluene	--	--	--	--	--	Toxicity value not available.
Nitrobenzene	--	--	--	--	--	Toxicity value not available.
Pentachloronitrobenzene	Chronic (35 weeks) NOAEL	Chicken	68,750	Not applicable	68,750	Dunn et al. (1979)
Phthalate esters (μg/kg BW-day)						
Bis(2-ethylhexyl)phthalate	Subchronic (4 weeks) NOAEL	Ring dove	1,110	0.1	111	Peakall (1974)
Di(n)octyl phthalate	--	--	--	--	--	Toxicity value not available.
Volatile organic compounds (μg/kg BW-day)						

TABLE E-8

BIRD TOXICITY REFERENCE VALUES

(Page 3 of 13)

Compound	Basis for TRV				TRV	Reference and Notes [d]
	Duration and Endpoint [a]	Test Organism	Dose[b]	Uncertainty Factor [c]		
Acetone	Acute (5 days) NOAEL	Coturnix quail	5,200,000	0.01[h]	52,000	Hill and Camardese (1986)
Acrylonitrile	--	--	--	--	--	Toxicity value not available.
Chloroform	--	--	--	--	--	Toxicity value not available.
Crotonaldehyde	--	--	--	--	--	Toxicity value not available.
1,4-Dioxane	--	--	--	--	--	Toxicity value not available.
Formaldehyde	--	--	--	--	--	Toxicity value not available.
Vinyl chloride	--	--	--	--	--	Toxicity value not available.
Other chlorinated organics (μg/kg BW-day)						
Hexachlorobenzene	Acute (5 days) NOAEL	Coturnix quail	22,500	0.01	225	Hill and Camardese (1986)
Hexachlorobutadiene	Chronic (3 months) NOAEL	Japanese quail	3185	Not applicable	3185	Schwertz et al. (1974)
Hexachlorocyclopentadiene	--	--	--	--	--	Toxicity value not available.
Pentachlorobenzene	--	--	--	--	--	Toxicity value not available.
Pentachlorophenol	Acute (5 days) NOAEL	Quail	403,000	0.01	4,030	Hill and Camardese (1986)
Pesticides (μg/kg BW-day)						
4,4'-DDE	Acute (5 days) LOAEL (mortality)	Coturnix quail	84,500	0.01	845	Hill and Camardese (1986). Test data for 1,1'-DDE used as a surrogate for 4,4'-DDE.

TABLE E-8

BIRD TOXICITY REFERENCE VALUES

(Page 4 of 13)

Compound	Basis for TRV				TRV	Reference and Notes [d]
	Duration and Endpoint [a]	Test Organism	Dose[b]	Uncertainty Factor [c]		
Heptachlor	Acute (5 days) LOAEL (mortality)	Quail	6,500	0.01	65	Hill and Camardese (1986)
Hexachlorophene	Acute LD50	Bobwhite quail	575,000	0.01	5,750	Meister (1994)
Inorganics (mg/kg BW-day)						
Aluminum	Chronic (4 -months) NOAEL (reproduction)	Ringed Turtle Dove	110	1.0	100	Carriere et al. (1986)
Antimony	--	--	--	--	--	Toxicity value not available. Ridgeway and Karnofsky (1952) reported LD50 for doses to eggs; however, that value could not be converted to a dose based on post-hatching environmental exposure.
Arsenic	Chronic (7 months) NOAEL	Brown-headed cowbird	2.46	1.0	2.46	U.S. Fish and Wildlife Service (1969)
Barium	Subchronic (4 weeks) NOAEL	One day old chick	208.26	0.1	20.8	Johnson et al. (1960)
Beryllium	--	--	--	--	--	Toxicity value not available.
Cadmium	Chronic (90 days) NOAEL	Mallard drake	1.45	Not applicable	1.45	White and Finley (1978)
Chromium (hexavalent)	Chronic (5 months) NOAEL	Black duck	1.0	Not applicable	1.0	Haseltine et al. (1985). TRV based on trivalent chromium.
Copper	Chronic (10 weeks) NOAEL (growth)	1-day old chicks	46.97	1.0	46.97	Mehring et al. (1960)

TABLE E-8

BIRD TOXICITY REFERENCE VALUES

(Page 5 of 13)

Compound	Basis for TRV				TRV	Reference and Notes [d]
	Duration and Endpoint [a]	Test Organism	Dose[b]	Uncertainty Factor [c]		
Total Cyanide	Acute LD50	American kestrel	4	0.01	0.04	Wiemeyer et al. (1986). Sodium cyanide is used as a surrogate for total cyanides.
Lead	Acute (7 days) LOAEL (altered enzyme levels)	Ringed turtle dove	25	0.001	0.025	Kendall and Scanlon (1982)
Mercuric chloride	Acute (5 days) LOAEL (mortality)	Coturnix quail	325	0.01	3.25	Hill and Camardese (1986)
Methyl mercury	Chronic (3 generations) LOAEL (mortality)	Mallard	0.064	0.1	0.0064	Heinz (1979)
Nickel	Subchronic (5 days) NOAEL	Coturnix quail	650	0.1	65	Hill and Camardese (1986)
Selenium	Chronic (78 days) NOAEL	Mallard	0.5	1.0	0.5	Heinz et al. (1987)
Silver	Subchronic (14 days) NOAEL	Mallard	1,780	0.1	178	U.S. EPA (1997)
Thallium	Acute LD50	Starling	35	0.01	0.35	Schafer (1972)
Zinc	Chronic (44 weeks) NOAEL	Leghorn hen and New Hampshire rooster	130.9	1.0	130.9	Stahl et al. (1990)

TABLE E-8

BIRD TOXICITY REFERENCE VALUES

(Page 6 of 13)

Notes:

a The duration of exposure is defined as chronic if it represents about 10 percent or more of the test animal's lifetime expectancy. Acute exposures represent single exposure or multiple exposures occurring within about two weeks or less. Subchronic exposures are defined as multiple exposures occurring for less than 10 percent of the test animal's lifetime expectancy but more that 2 weeks.

b Reported value which were dose in diet or water were converted to dose based on body weight and intake rate using Opresko, Sample, and Suter (1996).

c Uncertainty factors are used to extrapolate a reported toxicity value to a chronic NOAEL TRV. See Chapter 5 (Section 5.4) of the SLERAP for a discussion on the use of uncertainty factors. The TRV was calculated by multiplying the toxicity value by the uncertainty factor. A "not applicable" uncertainty factor is equivalent to a value equal to 1.0.

d The references refer to the study from which the endpoint and doses were identified. Complete reference citations are provided below.

e Best scientific judgement used to identify uncertainty factor. See Chapter 5 (Section 5.4.1.2) for a discussion on the use of best scientific judgement. Factors evaluated include test duration, ecological relevance of endpoint, experimental design, and availability of toxicity data.

HMW = High molecular weight
LOAEL = Lowest Observed Adverse Effect Level
LD50 = Concentration lethal to 50 percent of the test organisms.
NOAEL = No Observed Adverse Effect Level
TRV = Toxicity Reference Value

TABLE E-8

BIRD TOXICITY REFERENCE VALUES

(Page 7 of 13)

REFERENCES

Sample, Opresko, and Suter II (1996) provides a comprehensive review of bird toxicity information. This source was reviewed to identify studies to develop TRVs for birds. Based on the information presented, one or more references were obtained and reviewed to identify compound-specific toxicity values. For some compounds, the available information identified a single study meeting the requirements for a TRV, as discussed in Chapter 5 (Section 5.4) of the SLERAP. In most cases, each reference was obtained and reviewed to identify a single toxicity value to develop a TRV for each compound. As noted below, additional compendia were reviewed to identify toxicity studies to review. In a few cases where a primary study could not be obtained, a toxicity value is based on a secondary source. For compounds not discussed in Sample, Opresko, and Suter II (1996), the scientific literature was searched, and relevant studies were obtained and reviewed. The references reviewed are listed below. The study selected for the TRV is highlighted in bold.

Polychlorinated dibenzo(p)dioxins

Nosek, J.A., S.R. Craven, J.R. Sullivan, S.S. Hurley, and R.E. Peterson. 1992. "Toxicity and Reproductive Effects of 2,3,7,8-Tetrachlorodibenzo-p-dioxin in Ring-Necked Pheasant Hens." ***Journal of Toxicology and Environmental Health*****. Volume 35. Pages 187-198.**

U.S. EPA. 1993. *Interim Report on Data and Methods for Assessment of 2,3,7,8-Tetrachlorodibenzop-dioxin Risks to Aquatic Life and Associated Wildlife.* EPA/600/R-93/055. Office of Research and Development. Washington, D.C. March. This report identified the two studies listed below.

Greig, J.B., G. Jones, W.H. Butler, and J.M. Barnes. 1973. "Toxic Effects of 2,3,7,8-Tetrachlorodibenzo-p-dioxins. *Food and Cosmetics Toxicology*. Volume 11. Pages 585-595.

Hudson, R., R.Tucker, and M. Haegele. 1984. *Handbook of Toxicity of Pesticides to Wildlife.* Second Ed. U.S. Fish and Wildlife, Resources Publication No. 153. Washington, D.C.

Benzo(a)pyrene

Brunström, B., D. Broman, and C. Näf. 1991. "Toxicity and EROD-Inducing Potency of 24 Polycyclic Aromatic Hydrocarbons (PAHs) in Chick Embryos." ***Archives of Toxicology*****. Volume 65. Pages 485-489.**

Benzo(a)anthracene

Brunström, B., D. Broman, and C. Näf. 1991. "Toxicity and EROD-Inducing Potency of 24 Polycyclic Aromatic Hydrocarbons (PAHs) in Chick Embryos." ***Archives of Toxicology*****. Volume 65. Pages 485-489.**

Benzo(k)fluoranthene

Brunström, B., D. Broman, and C. Näf. 1991. "Toxicity and EROD-Inducing Potency of 24 Polycyclic Aromatic Hydrocarbons (PAHs) in Chick Embryos." *Archives of Toxicology*. Volume 65. Pages 485-489.

Chyrsene

Brunström, B., D. Broman, and C. Näf. 1991. "Toxicity and EROD-Inducing Potency of 24 Polycyclic Aromatic Hydrocarbons (PAHs) in Chick Embryos." *Archives of Toxicology*. Volume 65. Pages 485-489.

Dibenz(a,h)anthracene

Brunström, B., D. Broman, and C. Näf. 1991. "Toxicity and EROD-Inducing Potency of 24 Polycyclic Aromatic Hydrocarbons (PAHs) in Chick Embryos." *Archives of Toxicology*. Volume 65. Pages 485-489.

Indeno(1,2,3-cd)pyrene

Brunström, B., D. Broman, and C. Näf. 1991. "Toxicity and EROD-Inducing Potency of 24 Polycyclic Aromatic Hydrocarbons (PAHs) in Chick Embryos." *Archives of Toxicology*. Volume 65. Pages 485-489.

Polychlorinated Biphenyls

Peakall, D.B., J.L. Lincer, S.E. Bloom. 1972. "Embryonic Mortality and Chromosomal Alterations Caused by Aroclor 1254 in Ring Doves." *Environmental Health Perspectives*. Volume 1. Pages 103-104.

Dahlgren, R.B., R.L. Linder, and C.W. Carlson. 1972. "Polychlorinated Biphenyls: Their Effects on Penned Pheasants." *Environmental Health Perspectives*. Volume 1. Pages 89-101.

McLane, M.A.R., and D.L. Hughes. 1980. "Reproductive Success of Screech Owls Fed Aroclor 1248." *Archives of Environmental Contamination and Toxicolog*. Volume 9. Pages 661-665.

1,3-Dinitrobenzene

Schafer, E.W. 1972. "The Acute Oral Toxicity of 369 Pesticidal, Pharmaceutical and Other Chemicals to Wild Birds." *Toxicological and Applied Pharmacology*. Volume 21. Pages 315-330.

TABLE E-8

BIRD TOXICITY REFERENCE VALUES

(Page 9 of 13)

Pentachloronitrobenzene

Dunn, J. S., P. B. Bush, N. H. Booth, R.L. Farrell, D. M. Thomason, and D. D. Goetsch. 1979. Effect of Pentachloronitrobenzene upon Egg Production, Hatchability, and Residue Accumulation in the Tissues of White Leghorn Hens. *Toxicology and Applied Pharmacology*. Volume 48. Pages 425-433.

Bis(2-ethylhexyl)phthalate

Peakall, D.B. 1974. "Effects of Di-n-butyl and Di-2-ethylhexyl Phthalate on the Eggs of Ring Doves. *Bulletin of Environmental Contamination and Toxicology."* Volume 12. Pages 698-702.

Acetone

Hill, E.F., and M.B. Camardese. 1986. "Lethal Dietary Toxicities of Environmental Contaminants and Pesticides to Coturnix." Fish and Wildlife Service. Technical Report 2.

1,4-Dioxane

Giavini, E., C. Vismara, and L. Broccia. 1985. "Teratogenesis Study of Dioxane in Rats." *Toxicology Letters*. Volume 26. Pages 85-88. This study did not evaluate an ecologically relevant endpoint. Therefore, the data were not used to develop a TRV.

Hexachlorobenzene

Hill, E.F., and M.B. Camardese. 1986. "Lethal Dietary Toxicities of Environmental Contaminants and Pesticides to Coturnix." Fish and Wildlife Service. Technical Report 2.

Hexachlorobutadiene

Schwetz, B.A., J.M. Norris, R.J. Kociba, P.A. Keeler, R.F. Cornier, and P.J. Gehring. 1974. "Reproduction Study in Japanese Quail Fed Hexachlorobutadiene for 90 Days." *Toxicology and Applied Pharmacology*. Volume 30. Pages 255-265.

Pentachlorophenol

Hill, E.F., and M.B. Camardese. 1986. "Lethal Dietary Toxicities of Environmental Contaminants and Pesticides to Coturnix." Fish and Wildlife Service. Technical Report 2.

TABLE E-8

BIRD TOXICITY REFERENCE VALUES

(Page 10 of 13)

4,4'-DDE

Hill, E.F., and M.B. Camardese. 1986. "Lethal Dietary Toxicities of Environmental Contaminants and Pesticides to Coturnix." Fish and Wildlife Service. Technical Report 2.

Mendenhall, V.M., E.E. Klaas, and M.A.R. McLane. 1983. "Breeding Success of Barn Owls (*Tyto alba*) Fed Low Levels of DDE and Dieldrin." *Archives of Environmental Contamination and Toxicology*. *Volume*12. Pages 235-240.

Shellenberger, T.E. 1978. "A Multi-Generation Toxicity Evaluation of P-P'-DDT and Dieldrin with Japanese Quail. I. Effects on Growth and Reproduction." *Drug Chemistry and Toxicology*. *Volume* 1. Pages 137-146

Heptachlor

Hill, E.F., and M.B. Camardese. 1986. "Lethal Dietary Toxicities of Environmental Contaminants and Pesticides to Coturnix." Fish and Wildlife Service. Technical Report 2.

Hexachlorophene

Meister, R.J. (ed.) 1994. *Farm Chemicals Handbook '94*. Meister Publishing Company, Willoughby, Ohio. Volume 80. Page C189.

Aluminum

Carriere, D., K.L. Fischer, D.B. Peakall, and P. Anghern. 1986. "Effects of Dietary Aluminum Sulphate on Reproductive Success and Growth of Ringed Turtle Doves (*Streptopelia risoria*)." *Canadian Journal of Zoology*. Volume 64. Pages 1500-1505.

Carriere, D., K. Fischer, D. Peakall, and P. Angehrn. 1986. "Effects of Dietary Aluminum in Combination with Reduced Calcium and Phosphorus on the Ring Dove (*Streptopelia risoria*)." *Water, Air, and Soil Pollution*. Volume 30. Pages 757-764.

Antimony

Ridgeway, L.P. and D.A. Karnofsky. 1952. "The Effects of Metals on the Chick Embryo: Toxicity and Production of Abnormalities in Development." *Annals of New York Academy of Sciences*. Volume 55. Pages 203-215.

TABLE E-8

BIRD TOXICITY REFERENCE VALUES

(Page 11 of 13)

Arsenic

U.S. Fish and Wildlife Service. 1969. "Publication 74." Bureau of Sport Fisheries and Wildlife. As cited in Sample, Opresko, and Suter II (1996).

Barium

Johnson, D., Jr., A.L. Mehring, Jr., and H.W. Titus. 1960. "Tolerance of Chickens for Barium." *Proceedings o fthe Society for Experimental Biology and Medicine.* Volume 104. Pages 436-438.

Cadmium

White, D.H., and M.T. Finley. 1978. "Uptake and Retention of Dietary Cadmium in Mallard Ducks." *Environmental Research*. Volume 17. Pages 53-59.

Chromium

Haseltine, S.D., and others. 1985. "Effects of Chromium on Reproduction and Growth of Black Ducks." As cited in U.S. Fish and Wildlife Service. 1986. *Chromium Hazards to Fish, Wildlife, and Invertebrates: A Synoptic Review*. January. Page 38.

Copper

Mehring, A.L.Jr., J.H. Brumbaugh, A.J. Sutherland, and H.W. Titus. 1960. "The Tolerance of Growing Chickens for Dietary Copper." *Poultry Science.* Volume 39. Pages 713-719.

Cyanide

Wiemeyer, S.N., E.F. Hill, J.W. Carpenter, and A.J. Krynitsky. 1986. "Acute Oral Toxicity of Sodium Cyanide in Birds." *Journal of Wildlife Diseases*. Volume 22. Pages 538-46.

Lead

Kendall, R.J., and P.F. Scanlon. 1982. "The Toxicology of Ingested Lead Acetate in Ringed Turtle Doves *Stretopelia risoria*." *Environmental Pollution.* Volume 27. Pages 255-262.

Edens, F., W.E. Benton, S J. Bursian, and G.W. Morgan. 1976. "Effect of Dietary Lead on Reproductive Performance in Japanese Quail, *Coturnix coturnix japonica*." *Toxicology and Applied Pharmacology*. Volume 38. Pages 307-314.

Pattee, O.H. 1984. "Eggshell Thickness and Reproduction in American Kestrels Exposed to Chronic Dietary Lead." *Archives of Environmental Contamination and Toxicology*. Volume 13. Pages 29-34.

Mercuric chloride

Hill, E.F., and M.B. Camardese. 1986. "Lethal Dietary Toxicities of Environmental Contaminants and Pesticides to Coturnix." Fish and Wildlife Service. Technical Report 2.

Hill, E. F. and C. S. Schaffner. 1976. "Sexual Maturation and Productivity of Japanese Quail Fed Graded Concentrations of Mercuric Chloride." *Poultry Science.* Volume 55. Pages 1449-1459.

Methyl mercury

Heinz, G.H. 1979. "Methylmercury: Reproductive and Behavioral Effects on Three Generations of Mallard Ducks." *Journal of Wildlife Management*. Volume 43. Pages 394-401.

Spann, J.W., G.H. Heinz, M.B. Camardese, E.F. Hill, J.F. Moore, and H.C. Murray. 1986. "Differences in Mortality Among Bobwhite Fed Methylmercury Chloride Dissolved in Various Carriers." *Environmental Toxicology and Chemistry*. Volume 5. Pages 721-724.

Nickel

Hill, E.F., and M.B. Camardese. 1986. "Lethal Dietary Toxicities of Environmental Contaminants and Pesticides to Coturnix." Fish and Wildlife Service. Technical Report 2.

Cain, B.W., and E.A. Pafford. 1981. "Effects of Dietary Nickel on Survival and Growth of Mallard Ducklings." *Archives of Environmental Contamination and Toxicology*. Volume 10. Pages 737-745.

Selenium

Heinz, G., and others. 1987. "Research at Patuxent Wildlife Research Center." As cited in Sample, Opresko, and Suter II (1996).

Heinz, G.H., D.J. Hoffman, A.J. Krynitsky, and D.M.G. Weller. 1987. "Reproduction in Mallards Fed Selenium." *Environmental Toxicology and Chemistry*. Volume 6. Page 423-433.

TABLE E-8

BIRD TOXICITY REFERENCE VALUES

(Page 13 of 13)

Heinz, G.H., D.J. Hoffman, and L.G. Gold. 1989. "Impaired Reproduction of Mallards Fed an Organic Form of Selenium." *Journal of Wildlife Management*. Volume 53. Pages 418-428.

Sample, B.E., D.M. Opresko, G.W. Suter II. 1996. *Toxicological Benchmarks for Wildlife: 1996 Revision.* Risk Assessment Program Health Sciences Research Division, Oak Ridge, Tennessee. Prepared for U.S. Department of Energy.

Silver

U.S. EPA. 1997. Aquatic Toxicity Information Retrieval Database (AQUIRE). Office of Research and Development, National Health and Environmental Effects Research Laboratory, Mid-Continent Ecology Division. January.

Thallium

Schafer, E.W. 1972. "The Acute Oral Toxicity of 369 Pesticidal, Pharmaceutical and Other Chemicals to Wild Birds." *Toxicological and Applied Pharmacology*. Volume 21. Pages 315-330.

Zinc

Stahl, J.L., J.L. Greger, and M.E. Cook. 1990. "Breeding-Hen and Progeny Performance When Hens Are Fed Excessive Dietary Zinc." *Poultry Science*. Volume 69. Pages 259-263.

APPENDIX F

EQUATIONS FOR COMPUTING COPC CONCENTRATIONS AND COPC DOSE INGESTED TERMS

Screening Level Ecological Risk Assessment Protocol

August 1999

APPENDIX F

TABLE OF CONTENTS

Table **Page**

APPENDIX F

TABLE OF CONTENTS

APPENDIX F

TABLE OF CONTENTS

TABLE F-1-1

COPC CONCENTRATIONS IN TERRESTRIAL PLANTS FOR TERRESTRIAL FOOD WEBS

Description

This equation calculates the COPC concentration in plants due to: (1) *Pd* - wet and dry deposition of COPCs onto plant surfaces, (2) *Pv* - uptake of vapor phase COPCs onto plant surfaces, (3) *Pr* uptake of COPCs from soil through plant roots. Uncertainties associated with the use of this equation include the following:

Uncertainties introduced by this variable include the following:

(1) Some of the variables in the equations in Tables B-3-7, B-3-8, and B-3-9—including *Cs*, *Cyv*, *Q*, *Dydp*, and *Dywp*—are COPC- and site-specific. Uncertainties associated with these variables are site-specific.

(2) In the equation in Table B-3-7, uncertainties associated with other variables include the following: F_w (values for organic compounds estimated on the basis of the behavior of polystyrene microspheres), *Rp* (estimated on the basis of a generalized empirical relationship), *kp* (estimation process does not consider chemical degradation). All of these uncertainties contribute to the overall uncertainty associated with C_{TP}.

Equation

$$C_{TP} = (Pd + Pv + Pr)$$

Variable	Description	Units	Value
C_{TP}	COPC concentration in terrestrial plants	mg COPC/kg WW	

TABLE F-1-1

COPC CONCENTRATIONS IN TERRESTRIAL PLANTS FOR TERRESTRIAL FOOD WEBS

Variable	Description	Units	Value
Pd	Plant concentration due to direct deposition	mg COPC/kg WW	**Varies** This variable is calculated with the equation in Table B-3-1. This variable represents the COPC concentration in plants due to wet and dry deposition of COPCs onto plant surfaces. The limitations and uncertainty introduced in calculating this variable include the following: (1) Variables *Q*, *Dydp*, and *Dywp* are COPC- and site-specific. Uncertainties associated with these variables are site-specific. (2) In calculating the variable *Fw*, values of *r* assumed for most organic compounds—based on the behavior of insoluble polystyrene microspheres tagged with radionuclides— may accurately represent the behavior of organic compounds under site-specific conditions. (3) The empirical relationship used to calculate the variable *Rp*, and the empirical constant for use in the relationship, may not accurately represent site-specific plant types. (4) The recommended procedure for calculating the variable *kp* does not consider chemical degradation processes. This conservative approach contributes to the possible overestimation of plant concentrations.
Pv	Plant concentration due to air-to-plant transfer	mg COPC/kg WW	**Varies** This variable is calculated with the equation in Table B-3-2. Uncertainties associated with the use of this equation include the following: (1) The algorithm used to calculate values for the variable F_v assumes a default value for the parameter S_T (Whitby's average surface area of particulates [aerosols]) of background plus local sources, rather than an S_T value for urban sources. If a specific site is located in an urban area, the use of the latter S_T value may be more appropriate. The S_T value for urban sources is about one order of magnitude greater than that for background plus local sources and would result in a lower *Fv* value; however, the F_v value is likely to be only a few percent lower.
Pr	Plant concentration due to root uptake	mg COPC/kg WW	**Varies** This variable is calculated with the equation in Table B-3-3. *Cs* is the COPC concentration in soil due to deposition. This variable is calculated using emissions data, ISCST3 air dispersion and deposition model, and soil fate and transport equations (presented in Appendix B). Uncertainties associated with the use of this equation include the following: (1) The availability of site-specific information, such as meteorological data, will affect the accuracy of *Cs* estimates.

TABLE F-1-2

COPC CONCENTRATIONS IN HERBIVOROUS MAMMALS IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Description

This equation calculates the COPC concentration in herbivorous mammals through the ingestion of plants, soil, and water in the forest, shortgrass prairie, tallgrass prairie, and shrub/scrub food webs. The limitations and uncertainty introduced in calculating this variable include the following:

(1) Variables: C_{TP}, C_S, and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables are site-specific.
(2) Variables: $BCF_{TP\text{-}HM}$, $BCF_{S\text{-}HM}$ and $BCF_{W\text{-}HM}$ are based on biotransfer factors for beef cattle (Ba_{beef}), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations in site-specific herbivorous mammals.

Equation

$$C_{HM} = (C_{TP} \cdot BCF_{TP\text{-}HM} \cdot P_{TP} \cdot F_{TP}) + (C_S \cdot BCF_{S\text{-}HM} \cdot P_S) + (C_{wctot} \cdot BCF_{W\text{-}HM} \cdot P_W)$$

Variable	Description	Units	Value
C_{HM}	COPC concentration in herbivorous mammals	mg COPC/kg FW tissue	
C_{TP}	COPC concentration in terrestrial plants	mg COPC/kg WW	**Varies** This variable is site- and COPC-specific; it is calculated using the equation in Table F-1-1. Uncertainties introduced by this variable include the following: (1) Some of the variables in the equations in Tables B-3-1, B-3-2, and B-3-3—including *Cs*, *Cyv*, *Q*, *Dydp*, and *Dywp*—are COPC- and site-specific. (2) In the equation in Table B-3-1, uncertainties associated with other variables include the following: F_w (values for organic compounds estimated on the basis of the behavior of polystyrene microspheres), *Rp* (estimated on the basis of a generalized empirical relationship), and *kp* (estimation process does not consider chemical degradation). All of these uncertainties contribute to the overall uncertainty associated with C_{TP}. (3) In the equation in Table B-3-3, COPC-specific soil-to-plant bioconcentration factors (BCF_{TP}) may not reflect site-specific conditions.

TABLE F-1-2

COPC CONCENTRATIONS IN HERBIVOROUS MAMMALS IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
$BCF_{TP\text{-}HM}$	Bioconcentration factor for terrestrial plant-to-herbivorous mammal	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg WW)]	**Varies** This variable is COPC-, site-, and receptor-specific, and is calculated using the following equation to compute the COPC concentration in herbivorous mammals through dietary exposure. $BCF_{TP\text{-}HM}$ values are provided in Appendix D.
P_{TP}	Proportion of terrestrial plant in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{TP}	Fraction of diet comprised of terrestrial plants	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of terrestrial plants. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-1-2

COPC CONCENTRATIONS IN HERBIVOROUS MAMMALS IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_S	COPC concentration in soil	mg COPC /kg DW soil	**Varies** This variable is COPC- and site-specific, and should be calculated using the equation in Table B-1-1. This variable is calculated using emissions data, ISCST3 air dispersion and deposition model, and soil fate and transport equations (presented in Appendix B). C_S is expressed on a dry weight basis. Uncertainties associated with this variable include: (1) For soluble COPCs, leaching might lead to movement to below 1 centimeter in untilled soils, resulting a greater mixing depth. This uncertainty may overestimate *Cs*. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with *in situ* materials) in comparison to that of other residues. This uncertainty may underestimate *Cs*. (3) Modeled soil concentrations may not accurately represent site-specific conditions. As a result, the actual COPC concentration in soil may be under- or overestimated to an unknown degree.
$BCF_{S\text{-}HM}$	Bioconcentration factor for soil-to-herbivorous mammal	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg DW soil)]	**Varies** This variable is COPC-, site-, and receptor-specific, and is calculated using the following equation to compute the COPC concentration in herbivorous mammals through soil exposure. $BCF_{S\text{-}HM}$ values are provided in Appendix D.
P_S	Proportion of ingested soil that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor home range, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-1-2

COPC CONCENTRATIONS IN HERBIVOROUS MAMMALS IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values and may be significant in specific instances. Uncertainties associated with the variable L_T and K_{wt} may also be significant because of many variable-specific uncertainties. The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wtot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same media, the uncertainty associated with using default *OC* values may be significant in specific cases.
$BCF_{W\text{-}HM}$	Bioconcentration factor for water-to-herbivorous mammal pathways	unitless [(mg COPC/kg FW tissue)/(mg COPC/L water)]	**Varies** This variable is COPC-, site-, and receptor-specific, and is calculated using the following equation to compute the COPC concentration in herbivorous mammals through indirect water exposure (total water body concentration). $BCF_{W\text{-}HM}$ values are provided in Appendix D.

TABLE F-1-3

COPC CONCENTRATIONS IN INVERTEBRATES
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
P_W	Proportion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1.0** This OSW variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA recommend that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor home range, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

Description

This equation calculates the COPC concentration in invertebrates through exposure to soil in the forest, shortgrass prairie, tallgrass prairie, and shrub/scrub food webs. The limitations and uncertainty introduced in calculating this variable include the following:

(1) C_S values are COPC- and site-specific. Uncertainties associated with these variables are site specific.
(2) $BCF_{S\text{-}INV}$ values are intended to represent "generic invertebrate species", and therefore may over- or under-estimate exposure for site-specific organisms.

Equation

$$C_{INV} = C_S \cdot BCF_{S\text{-}INV}$$

Variable	Description	Units	Value
C_{INV}	COPC concentration in invertebrates	mg COPC/kg FW	

TABLE F-1-3

COPC CONCENTRATIONS IN INVERTEBRATES
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_S	COPC concentration in soil	mg COPC /kg DW soil	**Varies** This variable is COPC- and site-specific, and should be calculated using the equation in Table B-1-1. This variable is calculated using emissions data, ISCST3 air dispersion and deposition model, and soil fate and transport equations (presented in Appendix B). C_S is expressed on a dry weight basis. Uncertainties associated with this variable include: (1) For soluble COPCs, leaching might lead to movement to below 1 centimeter in untilled soils, resulting a greater mixing depth. This uncertainty may overestimate *Cs*. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with *in situ* materials) in comparison to that of other residues. This uncertainty may underestimate *Cs*. (3) Modeled soil concentrations may not accurately represent site-specific conditions. As a result, the actual COPC concentration in soil may be under- or overestimated to an unknown degree.
$BCF_{S\text{-}INV}$	Bioconcentration factor for soil-to-invertebrate	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg DW soil)]	**Varies** This variable is COPC-, site- and species-specific, and is provided in Appendix C. The following uncertainties are associated with this variable: (1) The COPC specific $BCF_{S\text{-}INV}$ values may not accurately represent site-specific soil conditions which could influence the bioavailability of COPCs, therefore over-or under-estimating C_{INV} to an unknown degree. (2) The data set used to calculate $BCF_{S\text{-}INV}$ is based on a limited number of test organism. The uncertainty associated with calculating concentrations using $BCF_{S\text{-}INV}$ in site-specific organisms is unknown and may over- or under-estimate C_{INV}.

TABLE F-1-4

COPC CONCENTRATIONS IN HERBIVOROUS BIRDS IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Description

This equation calculates the COPC concentration in herbivorous birds through the ingestion of plants, soil, and water in the forest, shortgrass prairie, tallgrass prairie, and shrub/scrub food webs. The limitations and uncertainty introduced in calculating this variable include the following:

(1) Variables: C_{TP}, C_S, and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables are site specific.
(2) Variables: $BCF_{TP\text{-}HB}$, $BCF_{S\text{-}HB}$, and $BCF_{W\text{-}HB}$ are calculated based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations in site-specific herbivorous birds.
(3) The use of a single $Ba_{chicken}$ value for each COPC may not accurately reflect site-specific conditions. The default values may under- or overestimate C_{HB}.

Equation

$$C_{HB} = (C_{TP} \cdot BCF_{TP\text{-}HB} \cdot P_{TP} \cdot F_{TP}) + (C_S \cdot BCF_{S\text{-}HB} \cdot P_S) + (C_{wctot} \cdot BCF_{W\text{-}HB} \cdot P_W)$$

Variable	Description	Units	Value
C_{HB}	COPC concentration in herbivorous birds	mg COPC/kg FW tissue	
C_{TP}	COPC concentration in terrestrial plants	mg COPC/kg WW	**Varies** This variable is site- and COPC-specific; it is calculated using the equation in Table F-1-1. Uncertainties introduced by this variable include the following: (1) Some of the variables in the equations in Tables B-3-1, B-3-2, and B-3-3—including *Cs, Cyv, Q, Dydp*, and *Dywp*—are COPC- and site-specific. (2) In the equation in Table B-3-1, uncertainties associated with other variables include the following: F_w (values for organic compounds estimated on the basis of the behavior of polystyrene microspheres), *Rp* (estimated on the basis of a generalized empirical relationship), and *kp* (estimation process does not consider chemical degradation). All of these uncertainties contribute to the overall uncertainty associated with C_{TP}.

TABLE F-1-4

COPC CONCENTRATIONS IN HERBIVOROUS BIRDS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
$BCF_{TP\text{-}HB}$	Bioconcentration factor for plant-to-herbivorous bird	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg WW)]	**Varies** This variable is COPC-, site-, habitat- and receptor-specific, and is calculated using the following equation to compute the COPC concentration in herbivorous birds through dietary exposure. $BCF_{TP\text{-}HB}$ values are porvided in Appendix D.
P_{TP}	Proportion of terrestrial plant in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{TP}	Fraction of diet comprised of terrestrial plants	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of terrestrial plants. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces significant uncertaintiy and may over-estimate exposure from ingestion of a single dietary item. (3) The defalut value for an equal diet introduces significant uncertainity and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-1-4

COPC CONCENTRATIONS IN HERBIVOROUS BIRDS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_S	COPC concentration in soil	mg COPC /kg DW soil	**Varies** This variable is COPC- and site-specific, and should be calculated using the equation in Table B-1-1. C_S is expressed on a dry weight basis. Uncertainties associated with this variable include: (1) For soluble COPCs, leaching might lead to movement to below 1 centimeter in untilled soils, resulting a greater mixing depth. This uncertainty may overestimate *Cs*. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with *in situ* materials) in comparison to that of other residues. This uncertainty may underestimate *Cs*. (3) Modeled soil concentrations may not accurately represent site-specific conditions. As a result, the actual COPC concentration in soil may be under- or overestimated to an unknown degree.
$BCF_{S\text{-}HB}$	Bioconcentration factor for soil-to-herbivorous bird	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg DW soil)]	**Varies** This variable is COPC-, site-, habitat- and receptor-specific, and is calculated using the following equation to compute the COPC concentration in herbivorous birds through soil exposure. $BCF_{S\text{-}HB}$ values are provided in Appendix D.
P_S	Proportion of ingested soil that is contamanted	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor home range, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-1-4

COPC CONCENTRATIONS IN HERBIVOROUS BIRDS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values and may be significant in specific instances. Uncertainties associated with the variable L_T and K_{wt} may also be significant because of many variable-specific uncertainties. The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wtot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same media, the uncertainty associated with using default *OC* values may be significant in specific cases.
$BCF_{W\text{-}HB}$	Bioconcentration factor for water-to-herbivorous bird	unitless [(mg COPC/kg FW tissue)/(mg COPC/L water)]	**Varies** This variable is COPC-, site-, and receptor-specific, and is calculated using the following equation to compute the COPC concentration in herbivorous birds through indirect exposure to water. $BCF_{W\text{-}HB}$ values are provided in Appendix D.
P_W	Proportion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

TABLE F-1-5

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS
IN FOREST, TALLGRASS PRAIRIE, SHORTGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Description

This equation calculates the COPC concentration in omnivorous mammals through ingestion of plants, soil, and water in the forest, shortgrass prairie, tallgrass prairie, and shrub/scrub food webs. The limitations and uncertainty introduced in calculating this variable include the following:

(1) Variables C_S, and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables are site specific.
(2) Variables: $BCF_{W\text{-}OM}$ and $BCF_{S\text{-}OM}$ are calculated based on biotransfer factors for beef cattle (Ba_{beef}), and receptor specific ingestion rates, and may introduce significant uncertainty when used to compute concentrations in site-specific omnivorous mammals.
(3) *FCMs* are COPC- and site-specific and may introduce uncertainty when applied to terrestrial environments to account for COPC bioaccumulation between trophic level (see Chapter 5 for further discussion).

Equation

$$C_{OM} = \left(C_{INV} \cdot \frac{FCM_{TL3}}{FCM_{TL2}} \cdot P_{INV} \cdot F_{INV}\right) + \left(C_{TP} \cdot BCF_{TP\text{-}OM} \cdot P_{TP} \cdot F_{TP}\right) + \left(C_{HM} \cdot \frac{FCM_{TL3}}{FCM_{TL2}} \cdot P_{HM} \cdot F_{HM}\right)$$

$$+ \left(C_{HB} \cdot \frac{FCM_{TL3}}{FCM_{TL2}} \cdot P_{HB} \cdot F_{HB}\right) + \left(C_S \cdot BCF_{S\text{-}OM} \cdot P_S\right) + \left(C_{wctot} \cdot BCF_{W\text{-}OM} \cdot P_W\right)$$

Variable	Description	Units	Value
C_{OM}	COPC concentration in omnivorous mammals	mg COPC/kg FW tissue	

TABLE F-1-5

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS
IN FOREST, TALLGRASS PRAIRIE, SHORTGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_{INV}	COPC concentration in invertebrates	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-3)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-3. Uncertainties associated with this variable include: (1) Modeled soil concentrations may not accurately represent site-specific conditions. As a result, the actual COPC concentration in soil used to calculate the COPC concentration in invertebrates may be under- or overestimated to an unknown degree. (2) $BCF_{S\text{-}INV}$ values may not accurately represent site-specific soil conditions and therefore, may over- or under-estimate C_{INV}.
$\frac{FCM_{TL3}}{FCM_{TL2}}$	Food chain multiplier for trophic level 3 predator consuming trophic level 2 prey	unitless	**Varies** This variable is COPC- and trophic level-specific and are provided in Chapter 5. The following uncertainties are associated with this variable: (1) *FCMs* do not account for metabolism, thus for COPCs with significant metabolism concentrations may be over-estimated to an unknown degree. (2) The application of *FCMs* for computing concentration in terrestrial food webs may introduce significant uncertainty (see Chapter 5) *FCMs* are obtained from the U.S. EPA (1995) "Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation Factors."
P_{INV}	Proportion of invertebrate in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.

TABLE F-1-5

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS
IN FOREST, TALLGRASS PRAIRIE, SHORTGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
F_{INV}	Fraction of diet comprised of invertebrates	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of invertebrates. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces significant uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces significant uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.
C_{TP}	COPC concentration in terrestrial plants ingested by the animal	mg COPC/kg WW	**Varies** This variable is site- and COPC-specific; it is calculated using the equation in Table F-1-1. Uncertainties introduced by this variable include the following: (1) Some of the variables in the equations in Tables B-3-1, B-3-2, and B-3-3—including *Cs*, *Cyv*, *Q*, *Dydp*, and *Dywp*—are COPC- and site-specific. (2) In the equation in Table B-3-1, uncertainties associated with other variables include the following: F_w (values for organic compounds estimated on the basis of the behavior of polystyrene microspheres), *Rp* (estimated on the basis of a generalized empirical relationship), *kp* (estimation process does not consider chemical degradation), and *Yp* (estimated on the basis of national harvest yield and area planted values). All of these uncertainties contribute to the overall uncertainty associated with C_{TP}. (3) In the equation in Table B-3-3, COPC-specific soil-to-plant bioconcentration factors (BCF_{TP}) may not reflect site-specific conditions.
$BCF_{TP\text{-}OM}$	Bioconcentration factor for terrestrial plant-to-omnivorous mammal	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg WW)]	**Varies** This variable is COPC-, site-, habitat- and receptor-specific, and is calculated using the following equation to compute the COPC concentration in omnivorous mammals through dietary exposure. $BCF_{TP\text{-}OM}$ values are provided in Appendix D.

TABLE F-1-5

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS
IN FOREST, TALLGRASS PRAIRIE, SHORTGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
P_{TP}	Proportion of terrestrial plant in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{TP}	Fraction of diet comprised of terrestrial plants	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of terrestrial plants. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.
C_{HM}	COPC concentration in herbivorous mammals	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-2)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-2. Uncertainties associated with this variable include: (1) Variables: C_{TP}, C_S, and C_{wctot} are COPC- and site-specific. (2) Variables: $BCF_{TP\text{-}HM}$, $BCF_{S\text{-}HM}$, and $BCF_{W\text{-}HM}$ are based on biotransfer factors for beef cattle (Ba_{beef}), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations in site-specific mammals.

TABLE F-1-5

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS
IN FOREST, TALLGRASS PRAIRIE, SHORTGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
P_{HM}	Proportion of herbivorous mammal in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{HM}	Fraction of diet comprised of herbivorous mammals	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of herbivorous mammal. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces significant uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces significant uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.
C_{HB}	COPC concentration in herbivorous birds	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-4)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-4. Uncertainties associated with this variable include: (1) Variables: C_{TP}, C_S, and C_{wctot} are COPC- and site-specific. (2) Variables: $BCF_{TP\text{-}HB}$, $BCF_{S\text{-}HB}$, and $BCF_{W\text{-}HB}$ are based on biotransfer factors for chicken ($Ba_{Chicken}$), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific herbivorous birds.

TABLE F-1-5

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS
IN FOREST, TALLGRASS PRAIRIE, SHORTGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
P_{HB}	Proportion of herbivorous birds in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{HB}	Fraction of diet comprised of herbivorous birds	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of herbivorous birds. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-1-5

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS
IN FOREST, TALLGRASS PRAIRIE, SHORTGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_S	COPC concentration in soil	mg COPC /kg DW soil	**Varies** This variable is COPC- and site-specific, and should be calculated using the equation in Table B-1-1. C_S is expressed on a dry weight basis. Uncertainties associated with this variable include: (1) For soluble COPCs, leaching might lead to movement to below 1 centimeter in untilled soils, resulting a greater mixing depth. This uncertainty may overestimate *Cs.* (2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with *in situ* materials) in comparison to that of other residues. This uncertainty may underestimate *Cs.* (3) Modeled soil concentrations may not accurately represent site-specific conditions. As a result, the actual COPC concentration in soil may be under- or overestimated to an unknown degree.
$BCF_{S\text{-}OM}$	Bioconcentration factor for soil-to-omnivorous mammal	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg DW soil)]	**Varies** This variable is COPC-, site-, and receptor-specific, and is calculated using the following equation to compute the COPC concentration in omnivorous mammals through indirect soil exposure. $BCF_{S\text{-}OM}$ values are provided in Appendix D.
P_S	Proportion of ingested soil that is contamanted	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor home range, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-1-5

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS
IN FOREST, TALLGRASS PRAIRIE, SHORTGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default *OC* content values and may be significant in specific instances. Uncertainties associated with the variable L_T and K_{wt} may also be significant because of many variable-specific uncertainties. The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wtot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same media, the uncertainty associated with using default *OC* values may be significant in specific cases.
$BCF_{W\text{-}OM}$	Bioconcentration factor for water-to-omnivorous mammal pathways	unitless [(mg COPC/kg FW tissue)/(mg COPC/L water)]	**Varies** This variable is COPC-, site-, and receptor-specific, and is calculated using the following equation to compute the COPC concentration in herbivorous mammals through indirect water exposure (total water body concentration). $BCF_{W\text{-}OM}$ values are provided in Appendix D.
P_W	Proportion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

TABLE F-1-5

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS
IN FOREST, TALLGRASS PRAIRIE, SHORTGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

REFERENCES AND DISCUSSIONS

U.S. EPA (1995) "Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation Factors."

TABLE F-1-6

COPC CONCENTRATIONS IN OMNIVOROUS BIRDS
IN FOREST, TALLGRASS PRAIRIE, SHORTGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Description

This equation calculates the COPC concentration in omnivorous birds through the ingestion of plants, soil, and water in the forest, shortgrass prairie, tallgrass prairie, and shrub/scrub food webs. The limitations and uncertainty introduced in calculating this variable include the following:

(1) Variables C_S, and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables are site specific.
(2) Variables: $BCF_{W\text{-}OB}$, and $BCF_{S\text{-}OB}$ are calculated based on biotransfer factors for chicken ($Ba_{Chicken}$), and receptor specific ingestion rates, and may introduce uncertainty when used to compute concentrations in site-specific omnivorous birds.
(3) *FCMs* are COPC- and site-specific and may introduce uncertainty when applied to terrestrial environments to account for COPC bioaccumulation between trophic (see Chapter 5).

Equation

$$C_{OB} = \left(C_{INV} \cdot \frac{FCM_{TL3}}{FCM_{TL2}} \cdot P_{INV} \cdot F_{INV}\right) + \left(C_{TP} \cdot BCF_{TP\text{-}OM} \cdot P_{TP} \cdot F_{TP}\right)$$

$$+ \left(C_S \cdot BCF_{S\text{-}OB} \cdot P_S\right) + \left(C_{wctot} \cdot BCF_{W\text{-}OB} \cdot P_W\right)$$

Variable	Description	Units	Value
C_{OB}	COPC concentration in omnivorous birds	mg COPC/kg FW tissue	
C_{INV}	COPC concentration in invertebrates	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-3)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-3. Uncertainties associated with this variable include: (1) Modeled soil concentrations may not accurately represent site-specific conditions. As a result, the actual COPC concentration in soil used to calculate the COPC concentration in invertebrates may be under- or overestimated to an unknown degree. (2) $BCF_{S\text{-}INV}$ values may not accurately represent site-specific soil conditions and therefore, may over- or under-estimate C_{INV}.

TABLE F-1-6

COPC CONCENTRATIONS IN OMNIVOROUS BIRDS
IN FOREST, TALLGRASS PRAIRIE, SHORTGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
$\underline{FCM}_{TL3}$ FCM_{TL2}	Food chain multiplier for trophic level 3 predator consuming trophic level 2 prey	unitless	**Varies** This variable is COPC- and trophic level-specific and is provided in Chapter 5 Table 5-2. The following uncertainties are associated with this variable: (1) *FCMs* do not account for metabolism, thus for COPCs with metabolism concentrations may be over-estimated to an unknown degree. (2) The application of *FCMs* for computing concentration in terrestrial food webs may introduce uncertainty (see Chapter 5) *FCMs* are obtained from the U.S. EPA 1995 "Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation Factors."
P_{INV}	Proportion of invertebrates in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.

TABLE F-1-6

COPC CONCENTRATIONS IN OMNIVOROUS BIRDS
IN FOREST, TALLGRASS PRAIRIE, SHORTGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
F_{INV}	Fraction of diet comprised of invertebrates	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of invertebrates. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.
C_{TP}	COPC concentration in terrestrial plants	mg COPC/kg WW	**Varies** This variable is site- and COPC-specific; it is calculated using the equation in Table F-1-1. Uncertainties introduced by this variable include the following: (1) Some of the variables in the equations in Tables B-3-1, B-3-2, and B-3-3—including *Cs*, *Cyv*, *Q*, *Dydp*, and *Dywp*—are COPC- and site-specific. (2) In the equation in Table B-3-1, uncertainties associated with other variables include the following: F_w (values for organic compounds estimated on the basis of the behavior of polystyrene microspheres), *Rp* (estimated on the basis of a generalized empirical relationship), *kp* (estimation process does not consider chemical degradation). All of these uncertainties contribute to the overall uncertainty associated with C_{TP}. (3) In the equation in Table B-3-3, COPC-specific soil-to-plant bioconcentration factors (BCF_{TP}) may not reflect site-specific conditions.
$BCF_{TP\text{-}OB}$	Bioconcentration factor for plant-to-omnivorous bird	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg WW)]	**Varies** This variable is COPC-, site-, habitat- and receptor-specific, and is calculated using the following equation to compute the COPC concentration in omnivorous birds through indirect dietary exposure. $BCF_{TP\text{-}OB}$ values are provided in Appendix D.

TABLE F-1-6

COPC CONCENTRATIONS IN OMNIVOROUS BIRDS
IN FOREST, TALLGRASS PRAIRIE, SHORTGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
P_{TP}	Proportion of terrestrial plant in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommend that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{TP}	Fraction of diet comprised of terrestrial plants	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of terrestrial plants. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-1-6

COPC CONCENTRATIONS IN OMNIVOROUS BIRDS
IN FOREST, TALLGRASS PRAIRIE, SHORTGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_S	COPC soil concentration	mg COPC /kg DW soil	**Varies** This variable is COPC- and site-specific, and should be calculated using the equation in Table B-1-1. C_S is expressed on a dry weight basis. Uncertainties associated with this variable include: (1) For soluble COPCs, leaching might lead to movement to below 1 centimeter in untilled soils, resulting a greater mixing depth. This uncertainty may overestimate *Cs*. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with *in situ* materials) in comparison to that of other residues. This uncertainty may underestimate *Cs*. (3) Modeled soil concentrations may not accurately represent site-specific conditions. As a result, the actual COPC concentration in soil may be under- or overestimated to an unknown degree.
$BCF_{S\text{-}OB}$	Bioconcentration factor for soil-to-omnivorous bird pathways	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg DW soil)]	**Varies** This variable is COPC-, site-, habitat- and receptor-specific, and is calculated using the following equation to compute the COPC concentration in omnivorous birds through indirect soil exposure. $BCF_{S\text{-}OB}$ values are provided in Appendix D.
P_S	Proportion of ingested soil that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor home range, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-1-6

COPC CONCENTRATIONS IN OMNIVOROUS BIRDS
IN FOREST, TALLGRASS PRAIRIE, SHORTGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values and may be significant in specific instances. Uncertainties associated with the variable L_T and K_{wt} may also be significant because of many variable-specific uncertainties. The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wtot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same media, the uncertainty associated with using default *OC* values may be significant in specific cases.
$BCF_{W\text{-}OB}$	Bioconcentration factor for water-to-omnivorous bird	unitless [(mg COPC/kg FW tissue)/(mg COPC/L water)]	**Varies** This variable is COPC-, site-, and receptor-specific, and is calculated using the following equation to compute the COPC concentration in omnivorous birds through indirect exposure to water. $BCF_{W\text{-}OB}$ values are provided in Appendix D.
P_W	Proportion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor home range, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

TABLE F-1-6

COPC CONCENTRATIONS IN OMNIVOROUS BIRDS IN FOREST, TALLGRASS PRAIRIE, SHORTGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

REFERENCES AND DISCUSSIONS

U.S. EPA 1995 “Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation Factors.”

TABLE F-1-7

COPC CONCENTRATIONS IN AQUATIC VEGETATION IN THE FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Description

This equation calculates the COPC concentration in aquatic vegetation through direct sediment exposure in the freshwater/wetland, brackish/intermediate marsh, and saltmarsh food webs. The limitations and uncertainty introduced in calculating this variable include the following:

(1) C_{sed} values are COPC- and site-specific. Uncertainties associated with these variables are site specific.
(2) $BCF_{W\text{-}AV}$ values are intended to represent "generic benthic invertebrate species", and therefore may over- or under-estimate exposure when applied to site-specific organisms.

Equation

$$C_{AV} = C_{sed} \cdot BCF_{S\text{-}AV}$$

Variable	Description	Units	Value
C_{AV}	COPC concentration in aquatic vegetation	mg COPC/kg WW	
C_{sed}	COPC concentration in bed sediment	mg COPC/kg DW sediment	**Varies (calculated - Table B-2-19)** This equation calculates the concentration of contaminants sorbed to bed sediments. Uncertainties associated with this equation include the following: (1) The default variable values recommended for use in the equation in Table B-2-19 may not accurately represent site-specific water body conditions. The degree of uncertainty associated with variables θ_{bs}, C_{sed}, d_{wc}, and d_{bs} is expected to be limited either because the probable ranges for these variables are narrow or because information allowing reasonable estimates is generally available. (2) Uncertainties associated with variables f_{bs}, C_{wctot} and Kd_{bs} are largely associated with the use of default *OC* content values in their calculation. The uncertainty may be significant in specific instances, because *OC* content is known to vary widely in different locations in the same medium. This variable is site-specific.

TABLE F-1-7

COPC CONCENTRATIONS IN AQUATIC VEGETATION IN THE FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
$BCF_{S\text{-}AV}$	Bioconcentration factor for sediment-to-aquatic vegetation	unitless [(mg COPC/kg WW)/(mg COPC/kg DW sediment)]	**Varies** This variable is COPC-, site- and species-specific, and is provided in Appendix C. This variable is calculated using laboratory and field measured values as discussed in Appendix C. The following uncertainties are associated with this variable: (1) The COPC specific $BCF_{S\text{-}AV}$ values may not accurately represent site-specific sediment conditions which could strongly influence the bioavailability of COPCs, therefore over-or under-estimating C_{AV} to an unknown degree. (2) The data set used to calculate $BCF_{S\text{-}AV}$ is based on soil-to-plant bioconcentration studies. The uncertainty associated with calculating concentrations using $BCF_{BS\text{-}AV}$ in site-specific organisms is unknown and may over- or under-estimate C_{AV}.

TABLE F-1-8

COPC CONCENTRATIONS IN ALGAE IN THE FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Description

This equation calculates the COPC concentration in algae through direct water exposure in the freshwater/wetland, brackish/intermediate marsh, and saltmarsh food webs. The limitations and uncertainty introduced in calculating this variable include the following:

(1) C_{dw} values are COPC- and site-specific. Uncertainties associated with these variables are site specific.
(2) $BCF_{W\text{-}AL}$ values are intended to represent "generic algae species", and therefore may over- or under-estimate exposure when applied to site-specific organisms.

Equation

$$C_{AL} = C_{dw} \cdot BCF_{W\text{-}AL}$$

Variable	Description	Units	Value
C_{AL}	COPC concentration in algae	mg COPC/kg WW	
C_{dw}	Dissolved phase water concentration	mg COPC/ L water	**Varies** This variable is COPC- and site-specific, and is calculated by using the equation in Table B-2-18. Uncertainties associated with this variable include the following: (1) The variables in the equation in Table B-2-18 are site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{dw}. The degree of uncertainty associated with *TSS* is expected to be relatively small, because information regarding reasonable site-specific values for this variable is generally available or can be easily measured. (2) The uncertainty associated with the variables C_{wctot} and Kd_{sw} is dependent on estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, the uncertainty associated with using different *OC* content values may be significant in specific cases.

TABLE F-1-8

COPC CONCENTRATIONS IN ALGAE IN THE FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
BCF_{WAL}	Bioconcentration factor for water-to-algae	unitless [(mg COPC/kg WW)/(mg COPC/L water)]	**Varies** This variable is COPC-, site- and species-specific, and is provided in Appendix C. This variable is computed using laboratory and field measured values as discussed in Appendix C. The following uncertainties are associated with this variable: (1) The COPC specific $BCF_{W\text{-}AL}$ values may not accurately represent site-specific sediment conditions, therefore over-or under-estimating C_{AL} to an unknown degree. (2) The data set used to calculate $BCF_{W\text{-}AL}$ is based on a limited number of test organisms. The uncertainty associated with calculating concentrations using $BCF_{W\text{-}AL}$ in site-specific organisms is unknown and may over- or under-estimate C_{AL}.

TABLE F-1-9

COPC CONCENTRATIONS IN HERBIVOROUS MAMMALS IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

(Page 1 of 5)

Description

This equation calculates the COPC concentration in aquatic herbivorous mammals through the ingestion of plants, sediment, and water in the freshwater/wetland, brackish/intermediate marsh, and saltmarsh food webs. The limitations and uncertainty introduced in calculating this variable include the following:

(1) Variables: C_{AV}, C_{sed}, and C_{wtot} are COPC- and site-specific. Uncertainties associated with these variables are site specific.
(2) Variables: $BCF_{TP\text{-}HM}$, $BCF_{bS\text{-}HM}$, and $BCF_{W\text{-}HM}$ are based on biotransfer factors for beef cattle (Ba_{beef}), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations in site-specific herbivorous mammals.
(3) The use of single Ba_{beef} value for each COPC may not accurately reflect site-specific conditions, and may under- or overestimate C_{HM}.

Equation

$$C_{HM} = (C_{AV} \cdot BCF_{HM} \cdot P_{AV} \cdot F_{AV}) + (C_{AL} \cdot BCF_{HM} \cdot P_{AL} \cdot F_{AL}) + (C_{sed} \cdot BCF_{BS\text{-}HM} \cdot P_{BS}) + (C_{wctot} \cdot BCF_{W\text{-}HM} \cdot P_{W})$$

Variable	Description	Units	Value
C_{HM}	COPC concentration in herbivorous mammals	mg COPC/kg FW tissue	
C_{AV}	COPC concentration in aquatic vegetation	mg COPC/kg WW	**Varies (calculated - Table F-1-7)** This variable is site- and COPC-specific; it is calculated using the equation in Table F-1-7. Uncertainties associated with this variable include: (1) C_{sed} values are COPC- and site-specific. (2) $BCF_{BS\text{-}AV}$ values are intended to represent "generic aquatic vegetation species", and therefore may over- or under-estimate exposure when applied to site-specific vegetation.
$BCF_{AV\text{-}HM}$	Bioconcentration factor for aquatic vegetation -to-aquatic herbivorous mammals	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg WW)]	**Varies** This variable is COPC-, site-, habitat- and receptor-specific, and is calculated using the following equation to compute the COPC concentration in aquatic herbivorous mammals through indirect dietary exposure. $BCF_{AV\text{-}HM}$ values are provided in Appendix D.

TABLE F-1-9

COPC CONCENTRATIONS IN HERBIVOROUS MAMMALS IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
P_{AV}	Proportion of aquatic vegetation in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{AV}	Fraction of diet comprised of aquatic vegetation	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic vegetation. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.
C_{AL}	COPC concentration in algae	mg COPC/kg WW	**Varies (calculated - Table F-1-8)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-8. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. (2) $BCF_{W\text{-}AL}$ values are intended to represent "generic algae species", and therefore may over- or under-estimate exposure when applied to site-specific species.

TABLE F-1-9

COPC CONCENTRATIONS IN HERBIVOROUS MAMMALS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
$BCF_{AL\text{-}HM}$	Bioconcentration factor for algae - to-aquatic herbivorous mammals	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg WW)]	**Varies** This variable is COPC-, site-, habitat- and receptor-specific, and is calculated using the following equation to compute the COPC concentration in aquatic herbivorous mammals through indirect dietary exposure. $BCF_{AL\text{-}HM}$ values are provided in Appendix D.
P_{AL}	Proportion of algae in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{AL}	Fraction of diet comprised of algae	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of algae. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-1-9

COPC CONCENTRATIONS IN HERBIVOROUS MAMMALS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{sed}	COPC concentration in bed sediment	mg COPC/kg DW sediment	**Varies (calculated - Table B-2-19)** This equation calculates the concentration of contaminants sorbed to bed sediments. Uncertainties associated with this equation include the following: (1) The default variable values recommended for use in the equation in Table B-2-19 may not accurately represent site-specific water body conditions. The degree of uncertainty associated with variables θ_{bs}, $C_{sed,\ wtotc}$, and d_{bs} is expected to be limited either because the probable ranges for these variables are narrow or because information allowing reasonable estimates is generally available. (2) Uncertainties associated with variables f_{bs}, C_{wtot} and Kd_{bs} are largely associated with the use of default *OC* content values in their calculation. The uncertainty may be significant in specific instances, because *OC* content is known to vary widely in different locations in the same medium. This variable is site-specific.
$BCF_{BS\text{-}HM}$	Bioconcentration factor for bed sediment-to-aquatic herbivorous mammal	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg DW sediment)]	**Varies** This variable is COPC-, site-, and receptor-specific, and is calculated using the following equation to compute the COPC concentration in aquatic herbivorous mammals through indirect sediment exposure. $BCF_{BS\text{-}HM}$ values are provided in Appendix D.
P_{BS}	Proportion of ingested bed sediment that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of sediment ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor home range, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-1-9

COPC CONCENTRATIONS IN HERBIVOROUS MAMMALS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values and may be significant in specific instances. Uncertainties associated with the variable L_T and K_{wt} may also be significant because of many variable-specific uncertainties. The degree of uncertainty associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wtot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same media, the uncertainty associated with using default *OC* values may be significant in specific cases.
$BCF_{W\text{-}HM}$	Bioconcentration factor for water-to-aquatic herbivorous mammal pathways	unitless [(mg COPC/kg FW tissue)/(mg COPC/L water)]	**Varies** This variable is COPC-, site-, and receptor-specific, and is calculated using the following equation to compute the COPC concentration in aquatic herbivorous mammals through indirect water exposure. $BCF_{W\text{-}HM}$ values are provided in Appendix D.
P_W	Proportion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor home range, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

TABLE F-1-10

COPC CONCENTRATIONS IN HERBIVOROUS BIRDS IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Description

This equation calculates the COPC concentration in aquatic herbivorous birds through ingestion of contaminated plants, sediment, and water in the freshwater/wetland, brackish/intermediate marsh, and saltmarsh food webs. The limitations and uncertainty introduced in calculating this variable include the following:

(1) Variables: C_{AV}, C_{sed}, and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables are site specific.
(2) Variables: $BCF_{AV\text{-}HB}$, $BCF_{BS\text{-}HB}$, and $BCF_{W\text{-}HB}$ are calculated based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific herbivorous birds.
(3) The use of single $Ba_{chicken}$ value for each COPC may not accurately reflect site-specific conditions; and may under- or overestimate C_{HB}.

Equation

$$C_{HB} = (C_{AV} \cdot BCF_{HB} \cdot P_{AV} \cdot F_{AV}) + (C_{AL} \cdot BCF_{HB} \cdot P_{AL} \cdot F_{AL}) + (C_{sed} \cdot BCF_{BS\text{-}HB} \cdot P_{BS}) + (C_{wctot} \cdot BCF_{W\text{-}HB} \cdot P_{W})$$

Variable	Description	Units	Value
C_{HB}	COPC concentration in herbivorous birds	mg COPC/kg FW tissue	
C_{AV}	COPC concentration in aquatic vegetation	mg COPC/kg WW	**Varies (calculated - Table F-1-7)** This variable is site- and COPC-specific; it is calculated using the equation in Table F-1-7. Uncertainties associated with this variable include: (1) C_{sed} values are COPC- and site-specific. (2) $BCF_{BS\text{-}AV}$ values are intended to represent "generic aquatic vegetation species", and therefore may over- or under-estimate exposure when applied to site-specific vegetation.
$BCF_{AV\text{-}HB}$	Bioconcentration factor for aquatic vegetation -to-aquatic herbivorous birds	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg WW)]	**Varies** This variable is COPC-, site-, habitat- and receptor-specific, and is calculated using the following equation to compute the COPC concentration in aquatic herbivorous birds through indirect dietary exposure. $BCF_{AV\text{-}HB}$ values are provided in Appendix D.

TABLE F-1-10

COPC CONCENTRATIONS IN HERBIVOROUS BIRDS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
P_{AV}	Proportion of aquatic vegetation in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{AV}	Fraction of diet comprised of aquatic vegetation	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic vegetation. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.
C_{AL}	COPC concentration in algae	mg COPC/kg WW	**Varies (calculated - Table F-1-8)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-8. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. (2) $BCF_{W\text{-}AL}$ values are intended to represent "generic algae species", and therefore may over- or under-estimate exposure when applied to site-specific species.

TABLE F-1-10

COPC CONCENTRATIONS IN HERBIVOROUS BIRDS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
BCF_{AL-HB}	Bioconcentration factor for algae - to-aquatic herbivorous birds	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg WW)]	**Varies** This variable is COPC-, site-, habitat- and receptor-specific, and is calculated using the following equation to compute the COPC concentration in aquatic herbivorous birds through indirect dietary exposure: BCF_{AL-HB} values are provided in Appendix D.
P_{AL}	Proportion of algae in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{AL}	Fraction of diet comprised of algae	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of algae. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-1-10

COPC CONCENTRATIONS IN HERBIVOROUS BIRDS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{sed}	COPC concentration in bed sediment	mg COPC/kg DW sediment	**Varies (calculated - Table B-2-19)** This equation calculates the concentration of COPSs in bed sediments. Uncertainties associated with this equation include the following: (1) The default variable values recommended for use in the equation in Table B-2-19 may not accurately represent site-specific water body conditions. The degree of uncertainty associated with variables θ_{bs}, $C_{sed,\ wtotc}$, and d_{bs} is expected to be limited either because the probable ranges for these variables are narrow or because information allowing reasonable estimates is generally available. (2) Uncertainties associated with variables f_{bs}, C_{wtot} and Kd_{bs} are largely associated with the use of default *OC* content values in their calculation. The uncertainty may be significant in specific instances, because *OC* content is known to vary widely in different locations in the same medium. This variable is site-specific.
$BCF_{BS\text{-}HB}$	Bioconcentration factor for bed sediment-to-aquatic herbivorous bird	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg DW sediment)]	**Varies** This variable is COPC-, site-, habitat- and receptor-specific, and is calculated using the following equation to compute the COPC concentration in aquatic herbivorous birds through indirect sediment exposure. $BCF_{BS\text{-}HB}$ values are provided in Appendix D.
P_{BS}	Proportion of ingested bed sediment that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor home range, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-1-10

COPC CONCENTRATIONS IN HERBIVOROUS BIRDS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default *OC* content values and may be significant in specific instances. Uncertainties associated with the variable L_T and K_{wt} may also be significant because of many variable-specific uncertainties. The degree of uncertainty associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wtot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, the uncertainty associated with using default *OC* values may be significant in specific cases.
$BCF_{W\text{-}HB}$	Bioconcentration factor for water-to-aquatic herbivorous bird	unitless [(mg COPC/kg FW tissue)/(mg COPC/L water)]	**Varies** This variable is COPC-, site-, and receptor-specific, and is calculated using the following equation to compute the COPC concentration in aquatic herbivorous birds through indirect exposure to water. $BCF_{W\text{-}HB}$ values are provided in Appendix D.
P_W	Proportion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor home range, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

TABLE F-1-11

COPC CONCENTRATIONS IN BENTHIC INVERTEBRATES IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Description

This equation calculates the COPC concentration in benthic invertebrates through direct exposure to benthic sediment in the freshwater/wetland, brackish/intermediate marsh, and saltmarsh food webs. The limitations and uncertainty introduced in calculating this variable include the following:

(1) C_{sed} values are COPC- and site-specific. Uncertainties associated with these variables are site specific.
(2) $BCF_{BS\text{-}BI}$ values are intended to represent "generic benthic invertebrate species", and therefore may over- or under-estimate exposure when applied to site-specific organisms.

Equation

$$C_{BI} = C_{sed} \cdot BCF_{BS-BI}$$

Variable	Description	Units	Value
C_{BI}	COPC concentration in benthic invertebrates	mg COPC/kg FW tissue	
C_{sed}	COPC concentration in bed sediment	mg COPC/kg DW sediment	**Varies (calculated - Table B-2-19)** This equation calculates the concentration of COPCs in bed sediments. Uncertainties associated with this equation include the following: (1) The default variable values recommended for use in the equation in Table B-2-19 may not accurately represent site-specific water body conditions. The degree of uncertainty associated with variables θ_{bs}, C_{sed}, d_{wc}, and d_{bs} is expected to be limited either because the probable ranges for these variables are narrow or because information allowing reasonable estimates is generally available. (2) Uncertainties associated with variables f_{bs}, C_{wtot} and Kd_{bs} are largely associated with the use of default *OC* content values in their calculation. The uncertainty may be significant in specific instances, because *OC* content is known to vary widely in different locations in the same medium. This variable is site-specific.

TABLE F-1-11

COPC CONCENTRATIONS IN BENTHIC INVERTEBRATES
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
$BCF_{BS\text{-}BI}$	Bioconcentration factor for sediment-to-benthic invertebrate	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg DW sediment)]	**Varies** This variable is COPC-, site- and species-specific, and is provided in Appendix C. This variable is calculated using laboratory and field measured values as discussed in Appendix C. The following uncertainties are associated with this variable: (1) The COPC specific $BCF_{BS\text{-}BI}$ values may not accurately represent site-specific sediment conditions which could strongly influence the bioavailability of COPCs, therefore over-or under-estimating C_{BI} to an unknown degree. (2) The data set used to calculate $BCF_{BS\text{-}BI}$ is based on a limited number of test organisms. The uncertainty associated with calculating concentrations using $BCF_{BS\text{-}BI}$ in site-specific organisms is unknown and may over- or under-estimate C_{BI}.

TABLE F-1-12

COPC CONCENTRATIONS IN WATER INVERTEBRATE IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Description

This equation calculates the COPC concentration in water invertebrates through direct water exposure in the freshwater/wetland, brackish/intermediate marsh, and saltmarsh food webs. The limitations and uncertainty introduced in calculating this variable include the following:

(1) C_{dw} values are COPC- and site-specific. Uncertainties associated with these variables are site specific.
(2) BCF_{WI} values are intended to represent "generic water invertebrate species", and therefore may over- or under-estimate exposure when applied to site-specific organisms.

Equation

$$C_{WI} = C_{dw} \cdot BCF_{W-WI}$$

Variable	Description	Units	Value
C_{WI}	COPC concentration in water invertebrates	mg COPC/kg FW tissue	
C_{dw}	Dissolved phase water concentration	mg COPC/L water	**Varies (calculated - Table B-2-18)** This variable is COPC- and site-specific. This equation calculates the concentration of COPC dissolved in the water column. Uncertainties associated with this equation include the following: (1) The variables in the equation in Table B-2-18 are site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{dw}. The degree of uncertainty associated with *TSS* is expected to be relatively small, because information regarding reasonable site-specific values for this variable are generally available or it can be easily measured. On the other hand, the uncertainty associated with the variables C_{wctot} and Kd_{sw} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, using default *OC* values may result in significant uncertainty in specific cases.

TABLE F-1-12

COPC CONCENTRATIONS IN WATER INVERTEBRATE
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
$BCF_{W\text{-}WI}$	Bioconcentration factor for water-to-invertebrate	unitless [(mg COPC/kg FW tissue)/(mg COPC/L water)]	**Varies** This variable is COPC-, site- and species-specific, and should be determined using Appendix C. This variable is calculated using laboratory and field measured values as discussed in Appendix C. The following uncertainties are associated with this variable: (1) The COPC specific $BCF_{W\text{-}WI}$ values may not accurately represent site-specific conditions, therefore over-or under-estimating C_{WI} to an unknown degree. (2) The data set used to calculate $BCF_{W\text{-}WI}$ is based on a limited number of test organisms. The uncertainty associated with calculating concentrations using $BCF_{W\text{-}WI}$ in site-specific organisms is unknown and may over- or under-estimate C_{WI}.

TABLE F-1-13

COPC CONCENTRATIONS IN HERBIVOROUS AND PLANKTIVOROUS FISH IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Description

This equation calculates the COPC concentration in herbivorous/planktivorous fish through ingestion of contaminated food and direct water exposure in the freshwater/wetland, brackish/intermediate marsh, and saltmarsh food webs. The limitations and uncertainty introduced in calculating this variable include the following:

(1) C_{dw} values are COPC- and site-specific. Uncertainties associated with these variables are site specific.
(2) The data set used to calculate BCF_f is based on a limited number of test organisms and therefore may over- or under-estimate exposure when applied to site-specific organisms.

Equation

$$C_{HF} = C_{dw} \cdot BCF_f \cdot FCM_{TL2}$$

Variable	Description	Units	Value
C_{HF}	COPC concentration in herbivorous and planktivorous fish	mg COPC/kg FW tissue	
C_{dw}	Dissolved phase water concentration	mg COPC/L water	**Varies (calculated - Table B-2-18)** This variable is COPC- and site-specific. This equation calculates the concentration of COPC dissolved in the water column. Uncertainties associated with this equation include the following: (1) The variables in the equation in Table B-2-18 are site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{dw}. The degree of uncertainty associated with *TSS* is expected to be relatively small, because information regarding reasonable site-specific values for this variable are generally available or it can be easily measured. On the other hand, the uncertainty associated with the variables C_{wctot} and Kd_{sw} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, using default *OC* values may result in significant uncertainty in specific cases.

TABLE F-1-13

COPC CONCENTRATIONS IN HERBIVOROUS AND PLANKTIVOROUS FISH IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
BCF_f	Bioconcentration factor for water-to-fish pathways	unitless [(mg COPC/kg FW tissue)/(mg COPC/L water)]	**Varies** This variable is COPC-, site- and species-specific, and is provided in Appendix C. This variable is calculated using laboratory and field measured values as discussed in Appendix C. The following uncertainties are associated with this variable: (1) The COPC specific BCF_f values may not accurately represent site-specific conditions, therefore over-or under-estimating C_{HF} to an unknown degree. (2) The data set used to calculate BCF_f is based on a limited number of test species. The uncertainty associated with calculating concentrations using BCF_f in site-specific organisms is unknown and may over- or under-estimate C_{HF}.
FCM_{TL2}	Food chain multiplier for trophic level 2 predator	unitless	**Varies** This variable is COPC- and trophic level-specific and is provided in Chapter 5, Table 5-2. The following uncertainties are associated with this variable: (1) *FCMs* do not account for metabolism, thus for COPCs with significant metabolism concentrations may be over-estimated to an unknown degree. (2) The application of *FCMs* for computing concentration in terrestrial food webs introduce uncertainty (see Chapter 5). *FCMs* are obtained from the U.S. EPA (1995) "Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation Factors."

TABLE F-1-13

COPC CONCENTRATIONS IN HERBIVOROUS AND PLANKTIVOROUS FISH IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

REFERENCES AND DISCUSSIONS

U.S. EPA. 1995. *Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation Factors.* Office of Water. EPA-820-B-95-005.

TABLE F-1-14

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Description

This equation calculates the COPC concentration in aquatic omnivorous mammals through ingestion of plants, sediment, and water in the freshwater/wetland, brackish/intermediate marsh, and saltmarsh food webs. The limitations and uncertainty introduced in calculating this variable include the following:

(1) Variables: C_{sed}, and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables are site specific.
(2) Variables: $BCF_{BS\text{-}OM}$, and $BCF_{W\text{-}OM}$ are based on biotransfer factors for beef cattle (Ba_{beef}), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations in site-specific omnivorous mammals.

Equation

$$C_{OM} = \left(C_{BI} \cdot \frac{FCM_{TL3}}{FCM_{TL2}} \cdot P_{BI} \cdot F_{BI}\right) + \left(C_{WI} \cdot \frac{FCM_{TL3}}{FCM_{TL2}} \cdot P_{WI} \cdot F_{WI}\right) + \left(C_{HM} \cdot \frac{FCM_{TL3}}{FCM_{TL2}} \cdot P_{HM} \cdot F_{HM}\right)$$

$$+ \left(C_{HB} \cdot \frac{FCM_{TL3}}{FCM_{TL2}} \cdot P_{HB} \cdot F_{HB}\right) + \left(C_{AL} \cdot BCF_{AL\text{-}OM} \cdot P_{AL} \cdot F_{AL}\right) + \left(C_{AV} \cdot BCF_{AV\text{-}OM} \cdot P_{AV} \cdot F_{AV}\right)$$

$$+ \left(C_{sed} \cdot BCF_{BS\text{-}OM} \cdot P_{BS}\right) + \left(C_{wctot} \cdot BCF_{W\text{-}OM} \cdot P_{W}\right)$$

Variable	Description	Units	Value
C_{OM}	COPC concentration in omnivorous mammals	mg COPC/kg FW tissue	

TABLE F-1-14

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{BI}	COPC concentration in benthic invertebrates	mg COPC/kg FW tissue	**Varies** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-11. Uncertainties associated with this variable include the following: (1) C_{sed} values are COPC- and site-specific. (2) $BCF_{BS\text{-}BI}$ values are intended to represent "generic benthic invertebrate species", and therefore may over- or under-estimate exposure when applied to site-specific organisms.
$\underline{FCM}_{TL3}$ FCM_{TL2}	Food chain multiplier for trophic level 3 predator consuming trophic level 2 prey	unitless	**Varies** This variable is COPC- and trophic level-specific and is provided in Chapter 5, Table 5-2. The following uncertainties are associated with this variable: (1) *FCMs* do not account for metabolism, thus for COPCs with significant metabolism, concentrations may be over-estimated to an unknown degree. (2) The application of *FCMs* for computing concentration in terrestrial food webs may introduce uncertainty (see Chapter 5) *FCMs* are obtained from the U.S. EPA 1995 "Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation Factors."
P_{BI}	Proportion of benthic invertebrate in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.

TABLE F-1-14

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
F_{BI}	Fraction of diet comprised of benthic invertebrates	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of benthic invertebrates. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.
C_{WI}	COPC concentration in water invertebrates	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-12)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-12. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. (2) $BCF_{W\text{-}WI}$ values are intended to represent "generic water invertebrate species", and therefore may over- or under-estimate exposure when applied to site-specific organisms.
P_{WI}	Proportion of water invertebrate in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.

TABLE F-1-14

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
F_{WI}	Fraction of diet comprised of water invertebrates	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of water invertebrates. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.
C_{HM}	Concentration of COPC in herbivorous mammals	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-9)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-9. Uncertainties associated with this variable include: (1) Variables: C_{AV}, C_{AL},C_{sed}, and C_{wctot} are COPC- and site-specific. (2) Variables: $BCF_{BS\text{-}HM}$ and $BCF_{W\text{-}HM}$ are based on biotransfer factors for beef cattle (Ba_{beef}), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific herbivorous mammals.
P_{HM}	Proportion of aquatic herbivorous mammal in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.

TABLE F-1-14

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
F_{HM}	Fraction of diet comprised of aquatic herbivorous mammals	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic herbivorous mammals. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.
C_{HB}	COPC concentration in herbivorous birds	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-10)** This variable is site-specific and chemical-specific; it is calculated using the equation in Table F-1-10. Uncertainties associated with this variable include: (1) Variables: C_{AV}, C_{AL},C_{sed}, and C_{wctot} are COPC- and site-specific. (2) Variables: $BCF_{BS\text{-}HB}$ and $BCF_{W\text{-}HB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific herbivorous birds.
P_{HB}	Proportion of herbivorous birds in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.

TABLE F-1-14

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
F_{HB}	Fraction of diet comprised of herbivorous birds	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic herbivorous birds. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.
C_{AL}	COPC concentration in algae	mg COPC/kg WW	**Varies (calculated - Table F-1-8)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-8. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. (2) $BCF_{W\text{-}AL}$ values are intended to represent "generic algae species", and therefore may over- or under-estimate exposure when applied to site-specific species.
$BCF_{AL\text{-}OM}$	Bioconcentration factor for algae-to-omnivorous mammal	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg WW)]	**Varies** This variable is COPC-, site-, habitat- and receptor-specific, and is calculated using the following equation to compute the COPC concentration in aquatic omnivorous mammals through indirect dietary exposure. $BCF_{AL\text{-}OM}$ values are provided in Appendix D.

TABLE F-1-14

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
P_{AL}	Proportion of algae in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{AL}	Fraction of diet comprised of algae	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of algae. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.
C_{AV}	COPC concentration in aquatic vegetation ingested by the animal	mg COPC/kg WW	**Varies (calculated - Table F-1-7)** This variable is site- and COPC-specific; it is calculated using the equation in Table F-1-7. Uncertainties associated with this variable include: (1) C_{sed} values are COPC- and site-specific. Uncertainties associated with this variable may be significant, and should be summarized as part of each SLERA report. (2) $BCF_{BS\text{-}AV}$ values are intended to represent "generic aquatic vegetation species", and therefore may over- or under-estimate exposure when applied to site-specific vegetation.

TABLE F-1-14

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
$BCF_{AV\text{-}OM}$	Bioconcentration factor for aquatic vegetation-to-aquatic omnivorous mammal	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg WW)]	**Varies** This variable is COPC-, site-, habitat- and receptor-specific, and is calculated using the following equation to compute the COPC concentration in aquatic omnivorous mammals through indirect dietary exposure. $BCF_{AV\text{-}OM}$ values are provided in Appendix D.
P_{AV}	Proportion of aquatic vegetation in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{AV}	Fraction of diet comprised of aquatic vegetation	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic vegetation. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-1-14

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{sed}	COPC concentration sorbed to bed sediment	mg COPC/kg DW sediment	**Varies (calculated - Table B-2-19)** This equation calculates the concentration of contaminants sorbed to bed sediments. Uncertainties associated with this equation include the following: (1) The default variable values recommended for use in the equation in Table B-2-19 may not accurately represent site-specific water body conditions. The degree of uncertainty associated with default variable values is expected to be limited either because the probable ranges for these variables are narrow or because information allowing reasonable estimates is generally available. (2) Uncertainties associated with variables f_{bs}, C_{wtot} and Kd_{bs} are largely associated with the use of default *OC* content values in their calculation. The uncertainty may be significant in specific instances, because *OC* content is known to vary widely in different locations in the same medium. This variable is site-specific.
$BCF_{BS\text{-}OM}$	Bioconcentration factor for bed sediment-to-aquatic omnivorous mammal pathways	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg DW sediment)]	**Varies** This variable is COPC-, site-, and receptor-specific, and is calculated using the following equation to compute the COPC concentration in aquatic omnivorous mammals through indirect sediment exposure. $BCF_{BS\text{-}OM}$ values are provided in Appendix D.
P_{BS}	Portion of ingested bed sediment that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor home range, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-1-14

COPC CONCENTRATIONS IN OMNIVOROUS MAMMALS IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default *OC* content values and may be significant in specific instances. Uncertainties associated with the variable L_T and K_{wt} may also be significant because of many variable-specific uncertainties. The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wtot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, the uncertainty associated with using default *OC* values may be significant in specific cases.
$BCF_{W\text{-}OM}$	Bioconcentration factor for water-to-aquatic omnivorous mammal	unitless [(mg COPC/kg FW tissue)/(mg COPC/L water)]	**Varies** This variable is COPC-, site-, and receptor-specific, and is calculated using the following equation to compute the COPC concentration in aquatic omnivorous mammals through indirect water exposure. $BCF_{W\text{-}OM}$ values are provided in Appendix D.
P_W	Portion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

TABLE F-1-15

COPC CONCENTRATIONS IN OMNIVOROUS BIRDS IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Description

This equation calculates the COPC concentration in aquatic omnivorous birds through ingestion of plants, sediment, and water in the freshwater/wetland, brackish/intermediate marsh, and saltmarsh food webs. The limitations and uncertainty introduced in calculating this variable include the following:

(1) Variables: C_{sed}, and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables are site specific.
(2) Variables: $BCF_{BS\text{-}OB}$, and $BCF_{W\text{-}OB}$ are calculated based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific omnivorous birds.

Equation

$$C_{OB} = \left(C_{BI} \cdot \frac{FCM_{TL3}}{FCM_{TL2}} \cdot P_{BI} \cdot F_{BI}\right) + \left(C_{WI} \cdot \frac{FCM_{TL3}}{FCM_{TL2}} \cdot P_{WI} \cdot F_{WI}\right) + \left(C_{AV} \cdot BCF_{AV\text{-}OM} \cdot P_{AV} \cdot F_{AV}\right)$$

$$+ \left(C_{AL} \cdot BCF_{AL\text{-}OM} \cdot P_{AL} \cdot F_{AL}\right) + \left(C_{sed} \cdot BCF_{BS\text{-}OB} \cdot P_{BS}\right) + \left(C_{wctot} \cdot BCF_{W\text{-}OB} \cdot P_{W}\right)$$

Variable	Description	Units	Value
C_{OB}	COPC concentration in omnivorous birds	mg COPC/kg FW tissue	
C_{BI}	COPC concentration in benthic invertebrates	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-11)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-11. Uncertainties associated with this variable include the following: (1) C_{sed} values are COPC- and site-specific. (2) $BCF_{BS\text{-}BI}$ values are intended to represent "generic benthic invertebrate species", and therefore may over- or under-estimate exposure when applied to site-specific organisms.

TABLE F-1-15

COPC CONCENTRATIONS IN OMNIVOROUS BIRDS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
$\frac{FCM_{TL3}}{FCM_{TL2}}$	Food chain multiplier for trophic level 3 predator consuming trophic level 2 prey	unitless	**Varies** This variable is COPC- and trophic level-specific and is provided in Chapter 5, Table 5-2. The following uncertainties are associated with this variable: (1) *FCMs* do not account for metabolism, thus for COPCs with significant metabolism, concentrations may be over-estimated to an unknown degree. (2) The application of *FCMs* for computing concentration in terrestrial food webs may introduce uncertainty (see Chapter 5) *FCMs* are obtained from the U.S. EPA 1995 "Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation Factors."
P_{BI}	Proportion of benthic invertebrate in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{BI}	Fraction of diet comprised of benthic invertebrates	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of benthic invertebrates. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-1-15

COPC CONCENTRATIONS IN OMNIVOROUS BIRDS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{WI}	COPC concentration in water invertebrates	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-12)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-12. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. (2) $BCF_{W\text{-}WI}$ values are intended to represent "generic water invertebrate species", and therefore may over- or under-estimate exposure when applied to site-specific organisms.
P_{WI}	Proportion of water invertebrate in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{WI}	Fraction of diet comprised of water invertebrates	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of water invertebrates. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-1-15

COPC CONCENTRATIONS IN OMNIVOROUS BIRDS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{AV}	COPC concentration in aquatic vegetation ingested by the animal	mg COPC/kg WW	**Varies (calculated - Table F-1-7)** This variable is site- and COPC-specific; it is calculated using the equation in Table F-1-7. Uncertainties associated with this variable include: (1) $C_{sed\text{-}AV}$ values are COPC- and site-specific. (2) $BCF_{BS\text{-}AV}$ values are intended to represent "generic aquatic vegetation species", and therefore may over- or under-estimate exposure when applied to site-specific vegetation.
$BCF_{AV\text{-}OB}$	Bioconcentration factor for aquatic vegetation-to-aquatic omnivorous bird	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg WW)]	**Varies** This variable is COPC-, site-, habitat- and receptor-specific, and is calculated using the following equation to compute the COPC concentration in aquatic omnivorous birds through indirect dietary exposure. $BCF_{AV\text{-}OB}$ values are provided in Appendix D.
P_{AV}	Proportion of aquatic vegetation in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.

TABLE F-1-15

COPC CONCENTRATIONS IN OMNIVOROUS BIRDS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
F_{AV}	Fraction of diet comprised of aquatic vegetation	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic vegetation. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.
C_{AL}	COPC concentration in algae	mg COPC/kg WW	**Varies (calculated - Table F-1-8)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-8. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. (2) $BCF_{W\text{-}AL}$ values are intended to represent "generic algae species", and therefore may over- or under-estimate exposure when applied to site-specific species.
$BCF_{AL\text{-}OB}$	Bioconcentration factor for algae-to-aquatic omnivorous bird	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg WW)]	**Varies** This variable is COPC-, site-, habitat- and receptor-specific, and is calculated using the following equation to compute the COPC concentration in aquatic omnivorous birds through indirect dietary exposure. $BCF_{AL\text{-}OB}$ values are provided in Appendix D.

TABLE F-1-15

COPC CONCENTRATIONS IN OMNIVOROUS BIRDS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
P_{AL}	Proportion of algae in diet that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommend that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{AL}	Fraction of diet comprised of algae	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of algae. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-1-15

COPC CONCENTRATIONS IN OMNIVOROUS BIRDS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{sed}	COPC concentration in bed sediment	mg COPC/kg DW sediment	**Varies (calculated - Table B-2-19)** This equation calculates the concentration of contaminants sorbed to bed sediments. Uncertainties associated with this equation include the following: (1) The default variable values recommended for use in the equation in Table B-2-19 may not accurately represent site-specific water body conditions. The degree of uncertainty associated with default variable values is expected to be limited either because the probable ranges for these variables are narrow or because information allowing reasonable estimates is generally available. (2) Uncertainties associated with variables f_{bs}, C_{wtot} and Kd_{bs} are largely associated with the use of default *OC* content values in their calculation. The uncertainty may be significant in specific instances, because *OC* content is known to vary widely in different locations in the same medium. This variable is site-specific. It is the maximum COPC concentration in sediment in the assessment area and is computed from soil and surface water concentrations using the ISCST3 air dispersion and deposition model, and fate and transport equations presented in Chapter 3.
$BCF_{BS\text{-}HB}$	Bioconcentration factor for bed sediment-to-aquatic omnivorous bird pathways	unitless [(mg COPC/kg FW tissue)/(mg COPC/kg DW sediment)]	**Varies** This variable is COPC-, site-, habitat- and receptor-specific, and is calculated using the following equation to compute the COPC concentration in aquatic herbivorous birds through indirect sediment exposure. $BCF_{BS\text{-}OB}$ values are provided in Appendix D.
P_{BS}	Portion of ingested bed sediment that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor home range, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-1-15

COPC CONCENTRATIONS IN OMNIVOROUS BIRDS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values and may be significant in specific instances. Uncertainties associated with the variable L_T and K_{wt} may also be significant because of many variable-specific uncertainties. The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wtot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, the uncertainty associated with using default *OC* values may be significant in specific cases.
$BCF_{W\text{-}OB}$	Bioconcentration factor for water-to-aquatic omnivorous bird	unitless [(mg COPC/kg FW tissue)/(mg COPC/L water)]	**Varies** This variable is COPC-, site-, and receptor-specific, and is calculated using the following equation to compute the COPC concentration in aquatic omnivorous birds through indirect exposure to water. $BCF_{W\text{-}OB}$ values are provided in Appendix D.
P_W	Portion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1.0** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommend that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor home range, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

TABLE F-1-15

COPC CONCENTRATIONS IN OMNIVOROUS BIRDS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

REFERENCES AND DISCUSSIONS

U.S. EPA. 1995. *Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation Factors.* Office of Water. EPA-820-B-95-005.

TABLE F-1-16

COPC CONCENTRATIONS IN OMNIVOROUS FISH IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Description

This equation calculates the COPC concentration in omnivorous fish through ingestion of contaminated food and water exposure in the freshwater/wetland, brackish/intermediate marsh, and saltmarsh food webs. The limitations and uncertainty introduced in calculating this variable include the following:

(1) C_{dw} values are COPC- and site-specific.
(2) The data set used to calculate BCF_f is based on a limited number of test organisms and therefore may over- or under-estimate exposure when representing site-specific organisms.

Equation

$$C_{OF} = C_{dw} \cdot BCF_f \cdot FCM_{TL3}$$

Variable	Description	Units	Value
C_{OF}	COPC concentration in omnivorous fish	mg COPC/kg FW tissue	
C_{dw}	Dissolved phase water concentration	mg COPC/L water	**Varies (calculated - Table B-2-18)** This variable is COPC- and site-specific. This equation calculates the concentration of COPC dissolved in the water column. Uncertainties associated with this equation include the following: (1) The variables in the equation in Table B-2-18 are site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{dw}. The degree of uncertainty associated with *TSS* is expected to be relatively small, because information regarding reasonable site-specific values for this variable are generally available or it can be easily measured. On the other hand, the uncertainty associated with the variables C_{wctot} and Kd_{sw} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same media, using default *OC* values may result in uncertainty in specific cases.

TABLE F-1-16

COPC CONCENTRATIONS IN OMNIVOROUS FISH
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
BCF_f	Bioconcentration factor for water-to-fish	unitless [(mg COPC/kg FW tissue)/(mg COPC/L water)]	**Varies** This variable is COPC-, site- and species-specific, and is provided in Appendix C. This variable is calculated using laboratory and field measured values as discussed Appendix C. The following uncertainties are associated with this variable: (1) The COPC specific BCF_f values may not accurately represent site-specific conditions, therefore over-or under-estimating C_{OF} to an unknown degree. (2) The data set used to calculate BCF_f is based on a limited number of test species. The uncertainty associated with calculating concentrations using BCF_f in site-specific organisms is unknown and may over- or under-estimate C_{OF}.
FCM_{TL3}	Food chain multiplier for trophic level 3 predator	unitless	**Varies** This variable is COPC- and trophic level-specific, and is provided in Chapter 5, Table 5-2. The following uncertainties are associated with this variable: (1) FCMs do not account for metabolism, thus for COPCs with significant metabolism concentrations may be over-estimated to an unknown degree. (2) The application of *FCMs* for computing concentration in terrestrial food webs introduce uncertainty (see Chapter 5). *FCMs* are obtained from the U.S. EPA 1995 "Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation Factors."

TABLE F-1-16

COPC CONCENTRATIONS IN OMNIVOROUS FISH
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

REFERENCES AND DISCUSSIONS

U.S. EPA. 1995. *Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation Factors.* Office of Water. EPA-820-B-95-005.

TABLE F-1-17

COPC CONCENTRATIONS IN CARNIVOROUS FISH IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Description

This equation calculates the COPC concentration in carnivorous fish through ingestion of contaminated prey and water exposure in the freshwater/wetland, brackish/intermediate marsh, and saltmarsh food webs. The limitations and uncertainty introduced in calculating this variable include the following:

(1) C_{dw} values are COPC- and site-specific.
(2) The data set used to calculate BCF_f is based on a limited number of test organisms and therefore may over- or under-estimate exposure when representing site-specific organisms.

Equation

$$C_{CF} = C_{dw} \cdot BCF_f \cdot FCM_{TL4}$$

Variable	Description	Units	Value
C_{CF}	COPC concentration in carnivorous fish	mg COPC/kg FW tissue	**Varies** Tissue concentration is expressed on a wet weight basis (mg COPC/kg wet tissue).
C_{dw}	Dissolved phase water concentration	mg COPC/L water	**Varies (calculated - Table B-2-18)** This variable is COPC- and site-specific. This equation calculates the concentration of COPC dissolved in the water column. Uncertainties associated with this equation include the following: (1) The variables in the equation in Table B-2-18 are site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, may contribute to the under- or overestimation of C_{dw}. The uncertainty associated with the variables C_{wctot} and Kd_{sw} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same media, using default *OC* values may result in uncertainty in specific cases.

TABLE F-1-17

COPC CONCENTRATIONS IN CARNIVOROUS FISH
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
BCF_f	Bioconcentration factor for water-to-fish	unitless [(mg COPC/kg FW tissue)/(mg COPC/L water)]	**Varies** This variable is COPC-, site- and species-specific, and is provided in Appendix C. This variable is calculated using laboratory and field measured values as discussed in Appendix C. The following uncertainties are associated with this variable: (1) The COPC specific BCF_f values may not accurately represent site-specific conditions, therefore over-or under-estimating C_{CF} to an unknown degree. (2) The data set used to calculate BCF_f is based on a limited number of test species. The uncertainty associated with calculating concentrations using BCF_f in site-specific organisms is unknown and may over- or under-estimate C_{CF}.
FCM_{TL4}	Food chain multiplier for trophic level 4 predator	unitless	**Varies** This variable is COPC- and trophic level-specific and is provided in Chapter 5, Table 5-2. The following uncertainties are associated with this variable: (1) *FCMs* do not account for metabolism, thus for COPCs with significant metabolism concentrations may be over-estimated to an unknown degree. (2) The application of *FCMs* for computing concentration in terrestrial food webs introduce uncertainty (see Chapter 5). *FCMs* are obtained from the U.S. EPA 1995 "Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation Factors."

TABLE F-1-17

COPC CONCENTRATIONS IN CARNIVOROUS FISH
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

REFERENCES AND DISCUSSIONS

U.S. EPA. 1995. *Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation Factors.* Office of Water. EPA-820-B-95-005.

TABLE F-2-1

COPC DOSE INGESTED TERMS IN HERBIVOROUS MAMMALS IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Description

This equation calculates the daily dose through exposure to contaminated food or prey, soil, and water in herbivorous mammals in upland forest, shortgrass prairie, tallgrass prairie, and shrub/scrub food webs. The limitations and uncertainties introduced in calculating this variable include the following:

(1) Variables *Cs* and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables will be site specific.
(2) Variables $BCF_{S\text{-}HM}$ and $BCF_{W\text{-}HM}$ are based on biotransfer factors for beef cattle (Ba_{beef}), and receptor-specific ingestion rates, and therefore may introduce uncertainty when used to compute a daily dose for representative site-specific herbivorous mammals.

Equation

$$D_{HM} = \left(C_{TP} \cdot IR_{HM} \cdot P_{TP} \cdot F_{TP}\right) + \left(Cs \cdot IR_{S\text{-}HM} \cdot P_S\right) + \left(C_{wctot} \cdot IR_{W\text{-}HM} \cdot P_W\right)$$

Variable	Description	Units	Value
D_{HM}	Dose COPC ingested for herbivorous mammals	mg COPC/kg BW-day	
C_{TP}	COPC concentration in terrestrial plants	mg COPC/kg WW	**Varies** This variable is site- and COPC-specific; it is calculated using the equation in Table F-1-1. Uncertainties introduced by this variable include the following: (1) Some of the variables in the equations in Tables B-3-1, B-3-2, and B-3-3—including *Cs*, *Cyv*, *Q*, *Dydp*, and *Dywp*—are COPC- and site-specific. (2) In the equation in Table B-3-1, uncertainties associated with other variables include the following: F_w (values for organic compounds estimated on the basis of the behavior of polystyrene microspheres), *Rp* (estimated on the basis of a generalized empirical relationship), *kp* (estimation process does not consider chemical degradation). All of these uncertainties contribute to the overall uncertainty associated with C_{TP}.

TABLE F-2-1

COPC DOSE INGESTED TERMS IN HERBIVOROUS MAMMALS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
IR_{HM}	Food ingestion rate of herbivorous mammal	kg WW/kg BW-day	**Varies** Food ingestion rates (IR_{HM}) are site-, receptor-, and habitat-specific and are provided in Chapter 5, Table 5-1. (1) Food ingestion rates are influenced by several factors including: metabolic rate, energy requirements for growth and reproduction, and dietary composition. Ingestion rates are also influenced by ambient temperature, receptor activity level and body weight (U.S. EPA 1993). These factors introduce an unknown degree of uncertainty when used to estimate daily dose.
P_{TP}	Proportion of terrestrial plant in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{TP}	Fraction of diet comprised of terrestrial plants	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of terrestrial plants. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-1

COPC DOSE INGESTED TERMS IN HERBIVOROUS MAMMALS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
Cs	COPC concentration in soil	mg COPC /kg DW soil	**Varies** This variable is COPC- and site-specific, and should be calculated using the equation in Table B-1-1. C_S is expressed on a dry weight basis. Uncertainties associated with this variable include: (1) For soluble COPCs, leaching might lead to movement to below 1 centimeter in untilled soils, resulting a greater mixing depth. This uncertainty may overestimate *Cs*. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with *in situ* materials) in comparison to that of other residues. This uncertainty may underestimate *Cs* (3) Modeled soil concentrations may not accurately represent site-specific conditions. As a result, the actual COPC concentration in soil may be under- or overestimated to an unknown degree.
$IR_{S\text{-}HM}$	Soil ingestion rate of omnivorous mammal	kg DW/kg BW-day	**Varies** This variable is site-, receptor-, and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. Uncertainties associated with this variable include the following: (1) IR_S values may under- or over-estimate BCF_S when applied for site-specific organisms.
P_S	Proportion of ingested soil that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-2-1

COPC DOSE INGESTED TERMS IN HERBIVOROUS MAMMALS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values and may be significant in specific instances. Uncertainties associated with the variable L_T and k_{wt} may also be significant because of many variable-specific uncertainties. The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wctot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same media, using default *OC* values may result in uncertainty in specific cases.
$IR_{W\text{-}HM}$	Water ingestion rate of herbivorous mammal	L/kg BW-day	**Varies** This variable is receptor- and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. The following uncertainty is associated with this variable: (1) Water ingestion rates are strongly influenced by animal behavior and environmental factors and may over- or under- estimate $BCF_{W\text{-}HM}$ to an unknown degree.
P_W	Proportion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

TABLE F-2-2

COPC DOSE INGESTED TERMS IN HERBIVOROUS BIRDS
IN FOREST, SHRUB/SCRUB, SHORTGRASS PRAIRIE, AND TALLGRASS PRAIRIE FOOD WEBS

Description

This equation calculates the daily dose through exposure to contaminated food/prey, soil, and water in herbivorous birds in upland forest, shortgrass prairie, tallgrass prairie, and shrub/scrub food webs. The limitations and uncertainties introduced in calculating this variable include the following:

(1) Variables C_S, and C_{HB} are COPC- and site-specific. Uncertainties associated with these variables will be site-specific.
(2) Variables $BCF_{S\text{-}HB}$, and $BCF_{W\text{-}HB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute a daily dose representing site-specific herbivorous birds.

Equation

$$D_{HB} = \left(C_{TP} \cdot IR_{HB} \cdot P_{TP} \cdot F_{TP}\right) + \left(Cs \cdot IR_{S\text{-}HB} \cdot P_S\right) + \left(C_{wctot} \cdot IR_{W\text{-}HB} \cdot P_W\right)$$

Variable	Description	Units	Value
D_{HB}	Dose COPC ingested for herbivorous birds	mg/kg BW-day	
C_{TP}	Concentration of COPC in terrestrial plants ingested by the animal	mg COPC/kg WW	**Varies** This variable is site- and COPC-specific; it is calculated using the equation in Table F-1-1. Uncertainties introduced by this variable include the following: (1) Some of the variables in the equations in Tables B-3-1, B-3-2, and B-3-3—including *Cs*, *Cyv*, *Q*, *Dydp*, and *Dywp*—are COPC- and site-specific. Uncertainties associated with these variables may be significant, and should be summarized as part of each SLERA report. (2) In the equation in Table B-3-1, uncertainties associated with other variables include the following: F_w (values for organic compounds estimated on the basis of the behavior of polystyrene microspheres), *Rp* (estimated on the basis of a generalized empirical relationship), and *kp* (estimation process does not consider chemical degradation). All of these uncertainties contribute to the overall uncertainty associated with C_{TP}.

TABLE F-2-2

COPC DOSE INGESTED TERMS IN HERBIVOROUS BIRDS
IN FOREST, SHRUB/SCRUB, SHORTGRASS PRAIRIE, AND TALLGRASS PRAIRIE FOOD WEBS

Variable	Description	Units	Value
IR_{HB}	Food ingestion rate of herbivorous bird	kg WW/kg BW-day	**Varies** This variable is receptor-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are provided in Chapter 5, Table 5-1. Uncertainties associated with this variable include: (1) Food ingestion rates are influenced by several factors including: metabolic rate, energy requirements for growth and reproduction, and dietary composition. Ingestion rates are also influenced by ambient temperature, receptor activity level and body weight U.S. EPA (1993). These factors introduce an unknown degree of uncertainty when used to estimate daily dose. (2) IR values may over- or under- estimate exposure when applied to site-specific receptors.
P_{TP}	Proportion of terrestrial plant diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{TP}	Fraction of diet comprised of terrestrial plants	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of terrestrial plants. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertaintiy and may over-estimate exposure from ingestion of a single dietary item. (3) The defalut value for an equal diet introduces uncertainity and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-2

COPC DOSE INGESTED TERMS IN HERBIVOROUS BIRDS
IN FOREST, SHRUB/SCRUB, SHORTGRASS PRAIRIE, AND TALLGRASS PRAIRIE FOOD WEBS

Variable	Description	Units	Value
Cs	COPC soil concentration	mg COPC /kg DW soil	**Varies** This variable is COPC- and site-specific, and should be calculated using the equation in Table B-1-1. This variable is calculated from stack emissions using the ISCST3 air dispersion and deposition model and soil fate and transport equations presented in Appendix B. C_S is expressed on a dry weight basis. Uncertainties associated with this variable include: (1) For soluble COPCs, leaching might lead to movement to below 1 centimeter in untilled soils, resulting a greater mixing depth. This uncertainty may overestimate *Cs* and Cs_{tD}. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with *in situ* materials) in comparison to that of other residues. This uncertainty may underestimate *Cs* (3) Modeled soil concentrations may not accurately represent site-specific conditions. As a result, the actual COPC concentration in soil may be under- or overestimated to an unknown degree.
$IR_{S\text{-}HB}$	Soil ingestion rate for herbivorous bird	kg DW/kg BW-day	**Varies** This variable is site-, receptor-, and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. Uncertainties associated with this variable include the following: (1) IR_S values may under- or over-estimate BCF_S when applied for site-specific organisms.
P_S	Proportion of ingested soil that is contamanted	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-2-2

COPC DOSE INGESTED TERMS IN HERBIVOROUS BIRDS IN FOREST, SHRUB/SCRUB, SHORTGRASS PRAIRIE, AND TALLGRASS PRAIRIE FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-16)** This variable is COPC- and site-specific and is calculated using Table B-2-16. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-16. are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values and may be significant in specific instances. Uncertainties associated with the variable L_T and K_{wt} may also be significant because of many variable-specific uncertainties. The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wctot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, the uncertainty associated with using default *OC* values may be significant in specific cases.
$IR_{W\text{-}HB}$	Water ingestion rate for herbivorous bird	kg WW/kg BW-day	**Varies** This variable is receptor- and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. The following uncertainty is associated with this variable: (1) Water ingestion rates are strongly influenced by animal behavior and environmental factors and may over- or under- estimate $BCF_{W\text{-}HB}$ to an unknown degree.
P_W	Proportion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

TABLE F-2-2

COPC DOSE INGESTED TERMS IN HERBIVOROUS BIRDS
IN FOREST, SHRUB/SCRUB, SHORTGRASS PRAIRIE, AND TALLGRASS PRAIRIE FOOD WEBS

REFERENCES AND DISCUSSIONS

U.S. EPA. 1993. *Wildlife Exposure Factor Handbook.* Volumes I and II. Office of Research and Development. EPA/600/R-93/187a.

TABLE F-2-3

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS IN FOREST, SHRUB/SCRUB, SHORTGRASS PRAIRIE, AND TALLGRASS PRAIRIE FOOD WEBS

Description

This equation calculates the daily dose through exposure to contaminated food/prey, soil, and water in omnivorous mammals in upland forest, shortgrass prairie, tallgrass prairie, and shrub/scrub food webs. The limitations and uncertainties introduced in calculating this variable include the following:

(1) Variables C_s and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables will be site-specific.
(2) Variables $BCF_{S\text{-}OM}$, and $BCF_{W\text{-}OM}$ are based on biotransfer factors for beef cattle (Ba_{beef}), and receptor-specific ingestion rates, and therefore may introduce uncertainty when used to compute a representative daily dose for site-specific omnivorous mammals.

Equation

$$D_{OM} = \left(C_{HM} \cdot IR_{OM} \cdot P_{HM} \cdot F_{HM}\right) + \left(C_{HB} \cdot IR_{OM} \cdot P_{HB} \cdot F_{HB}\right) + \left(C_{INV} \cdot IR_{OM} \cdot P_{INV} \cdot F_{INV}\right) + \left(C_{TP} \cdot IR_{OM} \cdot P_{TP} \cdot F_{TP}\right) + \left(C_s \cdot IR_{S\text{-}OM} \cdot P_S\right) + \left(C_{wctot} \cdot IR_{W\text{-}OM} \cdot P_W\right)$$

Variable	Description	Units	Value
D_{OM}	Dose COPC ingested for omnivorous mammals	mg COPC/kg BW-day	
C_{HM}	Concentration of COPC in herbivorous mammals	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-2)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-9. Uncertainties associated with this variable include: (1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. (2) Variables $BCF_{S\text{-}HM}$ and $BCF_{W\text{-}HM}$ are based on biotransfer factors for beef cattle (Ba_{beef}), and receptor-specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific herbivorous mammals.

TABLE F-2-3

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS
IN FOREST, SHRUB/SCRUB, SHORTGRASS PRAIRIE, AND TALLGRASS PRAIRIE FOOD WEBS

Variable	Description	Units	Value
IR_{OM}	Food ingestion rate of omnivorous mammal	kg WW/kg BW-day	**Varies** This variable is receptor-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are provided in Chapter 5, Table 5-1. Uncertainties associated with this variable include: (1) Food ingestion rates are influenced by several factors including: metabolic rate, energy requirements for growth and reproduction, and dietary composition. Ingestion rates are also influenced by ambient temperature, receptor activity level and body weight U.S. EPA (1993). These factors introduce an unknown degree of uncertainty when used to estimate daily dose. (2) *IR* values may over- or under- estimate exposure when applied to site-specific receptors.
P_{HM}	Proportion of herbivorous mammal in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommend that a default value of 1.0 be used for all food types when site specific information is not available. Uncertainties associated with this variable include: The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{HM}	Fraction of diet comprised of herbivorous mammals	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of herbivorous mammals. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. The application of an equal diet is further discussed in section Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of herbivorous mammals depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. Therefore a default value of 100 percent for the exclusive diet, may over-estimate dietary exposure.

TABLE F-2-3

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS
IN FOREST, SHRUB/SCRUB, SHORTGRASS PRAIRIE, AND TALLGRASS PRAIRIE FOOD WEBS

Variable	Description	Units	Value
C_{HB}	Concentration of COPC in herbivorous birds	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-10)** This variable is site-specific and chemical-specific; it is calculated using the equation in Table F-1-10. Uncertainties associated with this variable include: (1) Variables: C_{sed}, and C_{wctot} are COPC- and site-specific. (2) Variables: $BCF_{S\text{-}HB}$ and $BCF_{W\text{-}HB}$ are based on biotransfer factors for beef cattle ($Ba_{chicken}$), and receptor-specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific herbivorous mammals.
P_{HB}	Proportion of herbivorous birds in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{HB}	Fraction of diet comprised of herbivorous birds	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of herbivorous birds. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-3

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS IN FOREST, SHRUB/SCRUB, SHORTGRASS PRAIRIE, AND TALLGRASS PRAIRIE FOOD WEBS

Variable	Description	Units	Value
C_{INV}	Concentration of COPC in invertebrates	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-3)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-3. Uncertainties associated with this variable include: (1) Modeled soil concentrations may not accurately represent site-specific conditions. As a result, the actual COPC concentration in soil used to calculate the COPC concentration in invertebrates may be under- or overestimated to an unknown degree. (2) $BCF_{S\text{-}INV}$ values may not accurately represent site-specific soil conditions and therefore, may over- or under-estimate C_{INV}.
P_{INV}	Proportion of invertebrate in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{INV}	Fraction of diet comprised of invertebrates	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of invertebrates. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-3

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS
IN FOREST, SHRUB/SCRUB, SHORTGRASS PRAIRIE, AND TALLGRASS PRAIRIE FOOD WEBS

Variable	Description	Units	Value
C_{TP}	COPC concentration in terrestrial plants	mg COPC/kg WW	**Varies** This variable is site- and COPC-specific; it is calculated using the equation in Table F-1-1. Uncertainties introduced by this variable include the following: (1) Some of the variables in the equations in Tables B-3-1, B-3-2, and B-3-3—including *Cs*, *Cyv*, *Q*, *Dydp*, and *Dywp*—are COPC- and site-specific. (2) In the equation in Table B-3-1, uncertainties associated with other variables include the following: F_w (values for organic compounds estimated on the basis of the behavior of polystyrene microspheres), *Rp* (estimated on the basis of a generalized empirical relationship), and *kp* (estimation process does not consider chemical degradation). All of these uncertainties contribute to the overall uncertainty associated with C_{TP}.
P_{TP}	Proportion of terrestrial plant in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{TP}	Fraction of diet comprised of terrestrial plants	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of terrestrial plants. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-3

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS
IN FOREST, SHRUB/SCRUB, SHORTGRASS PRAIRIE, AND TALLGRASS PRAIRIE FOOD WEBS

Variable	Description	Units	Value
Cs	COPC concentration in soil	mg COPC /kg DW soil	**Varies** This variable is COPC- and site-specific, and should be calculated using the equation in Table B-1-1. C_S is expressed on a dry weight basis. Uncertainties associated with this variable include: (1) For soluble COPCs, leaching might lead to movement to below 1 centimeter in untilled soils, resulting a greater mixing depth. This uncertainty may overestimate *Cs*. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with *in situ* materials) in comparison to that of other residues. This uncertainty may underestimate *Cs* (3) Modeled soil concentrations may not accurately represent site-specific conditions. As a result, the actual COPC concentration in soil may be under- or overestimated to an unknown degree.
$IR_{S\text{-}OM}$	Soil ingestion rate of omnivorous mammal	kg DW/kg BW-day	**Varies** This variable is site-, receptor-, and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. Uncertainties associated with this variable include the following: (1) IR_S values may under- or over-estimate BCF_S when applied for site-specific organisms.
P_S	Proportion of ingested soil that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-2-3

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS IN FOREST, SHRUB/SCRUB, SHORTGRASS PRAIRIE, AND TALLGRASS PRAIRIE FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values and may be significant in specific instances. Uncertainties associated with the variable L_T and K_{wt} may result because of many variable-specific uncertainties. The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wctot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same media, using default *OC* values may result in uncertainty in specific cases.
$IR_{W\text{-}OM}$	Water ingestion rate for omnivorous mammal	L/kg DW-day	**Varies** This variable is receptor- and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. The following uncertainty is associated with this variable: (1) Water ingestion rates are influenced by animal behavior and environmental factors and may over- or under-estimate $BCF_{W\text{-}OM}$ to an unknown degree.
P_W	Proportion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

TABLE F-2-3

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS
IN FOREST, SHRUB/SCRUB, SHORTGRASS PRAIRIE, AND TALLGRASS PRAIRIE FOOD WEBS

REFERENCES AND DISCUSSIONS

U.S. EPA. 1993. *Wildlife Exposure Factor Handbook.* Volumes I and II. Office of Research and Development. EPA/600/R-93/187a

TABLE F-2-4

COPC DOSE INGESTED TERMS IN OMNIVOROUS BIRDS IN FOREST, SHRUB/SCRUB, TALLGRASS PRAIRIE, AND SHORTGRASS PRAIRIE FOOD WEBS

Description

This equation calculates the daily dose through exposure to contaminated food/prey, soil, and water in omnivorous birds in upland forest, shortgrass prairie, tallgrass prairie, and shrub/scrub food webs. The limitations and uncertainties introduced in calculating this variable include the following:

(1) Variables C_s and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables will be site specific.
(2) Variables $BCF_{S\text{-}OB}$, and $BCF_{W\text{-}OB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute a daily dose for site-specific omnivorous birds.

Equation

$$D_{OB} = \left(C_{INV} \cdot IR_{OB} \cdot P_{INV} \cdot F_{INV}\right) + \left(C_{TP} \cdot IR_{OB} \cdot P_{TP} \cdot F_{TP}\right) + \left(C_s \cdot IR_{S\text{-}OB} \cdot P_S\right) + \left(C_{wctot} \cdot IR_{W\text{-}OB} \cdot P_W\right)$$

Variable	Description	Units	Value
D_{OB}	Dose COPC ingested for omnivorous birds	mg COPC/kg BW-day	
C_{INV}	Concentration of COPC in invertebrates	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-3)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-3. Uncertainties associated with this variable include: (1) Modeled soil concentrations may not accurately represent site-specific conditions. As a result, the actual COPC concentration in soil used to calculate the COPC concentration in invertebrates may be under- or overestimated to an unknown degree. (2) $BCF_{S\text{-}INV}$ values may not accurately represent site-specific soil conditions and therefore, may over- or under-estimate C_{INV}.

TABLE F-2-4

COPC DOSE INGESTED TERMS IN OMNIVOROUS BIRDS
IN FOREST, SHRUB/SCRUB, TALLGRASS PRAIRIE, AND SHORTGRASS PRAIRIE FOOD WEBS

Variable	Description	Units	Value
IR_{OB}	Food ingestion rate of omnivorous bird	kg WW/kg BW-day	**Varies** This variable is receptor-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are provided in Chapter 5, Table 5-1. Uncertainties associated with this variable include: (1) Food ingestion rates are influenced by several factors including: metabolic rate, energy requirements for growth and reproduction, and dietary composition. Ingestion rates are also influenced by ambient temperature, receptor activity level and body weight U.S. EPA (1993). These factors introduce an unknown degree of uncertainty when used to estimate daily dose. (2) IR values may over- or under- estimate exposure when applied to site-specific receptors.
P_{INV}	Proportion of invertebrate in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{INV}	Fraction of diet comprised of invertebrates	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of invertebrates. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-4

COPC DOSE INGESTED TERMS IN OMNIVOROUS BIRDS
IN FOREST, SHRUB/SCRUB, TALLGRASS PRAIRIE, AND SHORTGRASS PRAIRIE FOOD WEBS

Variable	Description	Units	Value
C_{TP}	COPC concentration in terrestrial plants	mg COPC/kg WW	**Varies** This variable is site- and COPC-specific; it is calculated using the equation in Table F-1-1. Uncertainties introduced by this variable include the following: (1) Some of the variables in the equations in Tables B-3-1, B-3-2, and B-3-3—including *Cs*, *Cyv*, *Q*, *Dydp*, and *Dywp*—are COPC- and site-specific. (2) In the equation in Table B-3-1, uncertainties associated with other variables include the following: F_w (values for organic compounds estimated on the basis of the behavior of polystyrene microspheres), *Rp* (estimated on the basis of a generalized empirical relationship), and *kp* (estimation process does not consider chemical degradation).
P_{TP}	Proportion of terrestrial plant in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{TP}	Fraction of diet comprised of terrestrial plants	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of terrestrial plants. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-4

COPC DOSE INGESTED TERMS IN OMNIVOROUS BIRDS
IN FOREST, SHRUB/SCRUB, TALLGRASS PRAIRIE, AND SHORTGRASS PRAIRIE FOOD WEBS

Variable	Description	Units	Value
Cs	COPC concentration in soil	mg COPC /kg DW soil	**Varies** This variable is COPC- and site-specific, and should be calculated using the equation in Table B-1-1. C_S is expressed on a dry weight basis. Uncertainties associated with this variable include: (1) For soluble COPCs, leaching might lead to movement to below 1 centimeter in untilled soils, resulting a greater mixing depth. This uncertainty may overestimate *Cs*. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with *in situ* materials) in comparison to that of other residues. This uncertainty may underestimate *Cs*. (3) Modeled soil concentrations may not accurately represent site-specific conditions. As a result, the actual
$IR_{S\text{-}OB}$	Soil ingestion rate for omnivorous bird	kg DW/kg BW-day	**Varies** This variable is site-, receptor-, and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. Uncertainties associated with this variable include the following: (1) IR_S values may under- or over-estimate BCF_S when applied to site-specific organisms.
P_S	Proportion of ingested soil that is contamanted	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site-specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated may be overestimated.

TABLE F-2-4

COPC DOSE INGESTED TERMS IN OMNIVOROUS BIRDS
IN FOREST, SHRUB/SCRUB, TALLGRASS PRAIRIE, AND SHORTGRASS PRAIRIE FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values and may be significant in specific instances. Uncertainties associated with the variable L_T and K_{wt} may also be significant because of many variable-specific uncertainties. The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wctot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same media, default *OC* values will result in uncertainty in specific cases.
$IR_{W\text{-}OB}$	Water ingestion rate for omnivorous bird	L/kg BW-day	**Varies** This variable is receptor- and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. The following uncertainty is associated with this variable: (1) Water ingestion rates are influenced by animal behavior and environmental factors and may over- or under-estimate $BCF_{W\text{-}OB}$ to an unknown degree.
P_W	Proportion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated may be overestimated.

TABLE F-2-4

COPC DOSE INGESTED TERMS IN OMNIVOROUS BIRDS
IN FOREST, SHRUB/SCRUB, TALLGRASS PRAIRIE, AND SHORTGRASS PRAIRIE FOOD WEBS

REFERENCES AND DISCUSSIONS

U.S. EPA. 1993. *Wildlife Exposure Factor Handbook.* Volumes I and II. Office of Research and Development. EPA/600/R-93/187a.

TABLE F-2-5

COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Description

This equation calculates the daily dose through exposure to food/prey, soil, and water in carnivorous mammal in upland forest, shortgrass prairie, tallgrass prairie, and shrub/scrub food webs. The limitations and uncertainties introduced in calculating this variable include the following:

(1) Variables C_s and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables will be site-specific
(2) Variables $BCF_{S\text{-}CM}$, and $BCF_{W\text{-}CM}$ are based on biotransfer factors for beef cattle (Ba_{beef}), and receptor-specific ingestion rates, and therefore may introduce uncertainty when used to compute a representative daily dose for site-specific carnivorous mammals.

Equation

$$D_{CM} = \left(C_{HB} \cdot IR_{CM} \cdot P_{HB} \cdot F_{HB}\right) + \left(C_{OB} \cdot IR_{CM} \cdot P_{OB} \cdot F_{OB}\right) + \left(C_{OM} \cdot IR_{CM} \cdot P_{OM} \cdot F_{OM}\right) + \left(C_{HM} \cdot IR_{CM} \cdot P_{HM} \cdot F_{HM}\right) + \left(C_s \cdot IR_{S\text{-}CM} \cdot P_S\right) + \left(C_{wctot} \cdot IR_{W\text{-}CM} \cdot P_W\right)$$

Variable	Description	Units	Value
D_{CM}	Dose COPC ingested for carnivorous mammals	mg COPC/kg BW-day	
C_{HB}	Concentration of COPC in herbivorous birds	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-10)** This variable is site-specific and chemical-specific; it is calculated using the equation in Table F-1-10. Uncertainties associated with this variable include: (1) Variables *Cs* and C_{wctot} are COPC- and site-specific. (2) Variables $BCF_{S\text{-}HB}$ and $BCF_{W\text{-}HB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor-specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific herbivorous birds.

TABLE F-2-5

COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
IR_{CM}	Food ingestion rate of carnivorous mammal	kg WW/kg BW-day	**Varies** This variable is receptor-specific, and is discussed in Chapter 5, Table 5-1. Uncertainties associated with this variable include: (1) Food ingestion rates are influenced by several factors including: metabolic rate, energy requirements for growth and reproduction, and dietary composition. Ingestion rates are also influenced by ambient temperature, receptor activity level and body weight U.S. EPA (1993). These factors introduce an unknown degree of uncertainty when used to estimate daily dose. (2) *IR* values may over- or under- estimate exposure when applied for site-specific receptors.
P_{HB}	Proportion of herbivorous birds in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{HB}	Fraction of diet comprised of herbivorous birds	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of herbivorous birds. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-5

COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_{OB}	Concentration of COPC in omnivorous birds	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-6)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-6. Uncertainties associated with this variable include: (1) Variables *Cs* and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables will be site-specific. (2) Variables $BCF_{S\text{-}OB}$ and $BCF_{W\text{-}OB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor-specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific omnivorous birds.
P_{OB}	Proportion of omnivorous bird diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommend that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{OB}	Fraction of diet comprised of omnivorous birds	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of omnivorous birds. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-5

COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_{OM}	Concentration of COPC in omnivorous mammals	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-5)** This variable is site-specific and COPC-specific, and is calculated using the equation in Table F-1-5. Uncertainties associated with this variable include: (1) Variables *Cs* and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables will be site-specific. (2) Variables $BCF_{S\text{-}OM}$ and $BCF_{W\text{-}OM}$ are based on biotransfer factors for beef (Ba_{beef}), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific omnivorous mammals.
P_{OM}	Proportion of omnivorous mammal diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{OM}	Fraction of diet comprised of omnivorous mammals	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of omnivorous mammals. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-5

COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_{HM}	Concentration of COPC in herbivorous mammals	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-9)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-9. Uncertainties associated with this variable include: (1) Variables *Cs* and C_{wctot} are COPC- and site-specific. (2) Variables $BCF_{S\text{-}HM}$ and $BCF_{W\text{-}HM}$ are based on biotransfer factors for beef cattle (Ba_{beef}), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific herbivorous mammals.
P_{HM}	Proportion of herbivorous mammal in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommend that a default value of 1.0 be used for all food types when site specific information is not available. Uncertainties associated with this variable include: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{HM}	Fraction of diet comprised of herbivorous mammals	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of herbivorous mammals. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of herbivorous mammals depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. Therefore a default value of 100 percent for the exclusive diet, may over-estimate dietary exposure.

TABLE F-2-5

COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
Cs	COPC concentration in soil	mg COPC /kg DW soil	**Varies** This variable is COPC- and site-specific, and should be calculated using the equation in Table B-1-1. *Cs* is expressed on a dry weight basis. Uncertainties associated with this variable include: (1) For soluble COPCs, leaching might lead to movement to below 1 centimeter in untilled soils, resulting a greater mixing depth. This uncertainty may overestimate *Cs*. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with *in situ* materials) in comparison to that of other residues. This uncertainty may underestimate *Cs* (3) Modeled soil concentrations may not accurately represent site-specific conditions. As a result, the actual COPC concentration in soil may be under- or overestimated to an unknown degree.
$IR_{S\text{-}CM}$	Soil ingestion rate for carnivorous mammal	kg DW/kg BW-day	**Varies** This variable is site-, receptor-, and habitat-specific, and is discussed in Chapter 5; Table 5-1. Uncertainties associated with this variable include the following: (1) IR_S values may under- or over-estimate BCF_S when applied to site-specific organisms.
P_S	Proportion of ingested soil that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated may be overestimated.

TABLE F-2-5

COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values. Uncertainties may also be associated with the variable L_T and K_{wt}. The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wctot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, the uncertainty associated with using default *OC* values may be significant in specific cases.
$IR_{W\text{-}CM}$	Water ingestion rate for carnivorous mammal	L/kg BW-day	**Varies** This variable is receptor- and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in, Table 5-1. The following uncertainty is associated with this variable: (1) Water ingestion rates are strongly influenced by animal behavior and environmental factors and may over- or under- estimate $BCF_{W\text{-}CM}$ to an unknown degree.
P_W	Proportion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated may be overestimated.

TABLE F-2-5

COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

REFERENCES AND DISCUSSIONS

U.S. EPA. 1993. *Wildlife Exposure Factor Handbook.* Volumes I and II. Office of Research and Development. EPA/600/R-93/187a

TABLE F-2-6

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Description

This equation calculates the potential daily dose through exposure to contaminated food/prey, soil, and water in carnivorous birds in upland forest, shortgrass prairie, tallgrass prairie, and shrub/scrub food webs. The limitations and uncertainties introduced in calculating this variable include the following:

(1) Variables *Cs* and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables will be site-specific.
(2) Variables $BCF_{S\text{-}CB}$ and $BCF_{W\text{-}CB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor-specific ingestion rates, and therefore may introduce uncertainty when used to compute a representative daily dose for site-specific carnivorous birds.

Equation

$$D_{CB} = \left(C_{HB} \cdot IR_{CB} \cdot P_{HB} \cdot F_{HB}\right) + \left(C_{OM} \cdot IR_{CB} \cdot P_{OM} \cdot F_{OM}\right) + \left(C_{HM} \cdot IR_{CB} \cdot P_{HM} \cdot F_{HM}\right)$$
$$+ \left(C_{OB} \cdot IR_{CB} \cdot P_{OB} \cdot F_{OB}\right) + \left(C_{s} \cdot IR_{S\text{-}CB} \cdot P_{S}\right) + \left(C_{wctot} \cdot IR_{W\text{-}CB} \cdot P_{W}\right)$$

Variable	Description	Units	Value
D_{CB}	Dose COPC ingested for carnivorous birds	mg COPC/kg BW-day	
C_{HB}	Concentration of COPC in herbivorous birds	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-10)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-10. Uncertainties associated with this variable include: (1) Variables *Cs* and C_{wctot} are COPC- and site-specific. (2) Variables $BCF_{S\text{-}HB}$ and $BCF_{W\text{-}HB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor-specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific herbivorous birds.

TABLE F-2-6

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
IR_{CB}	Food ingestion rate of carnivorous bird	kg WW/kg DW-day	**Varies** This variable is receptor-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are provided in Table 5-1. Uncertainties associated with this variable include: (1) Food ingestion rates are influenced by several factors including: metabolic rate, energy requirements for growth and reproduction, and dietary composition. Ingestion rates are also influenced by ambient temperature, receptor activity level and body weight U.S. EPA (1993). These factors introduce an unknown degree of uncertainty when used to estimate daily dose. (2) IR values may over- or under- estimate exposure when applied for site-specific receptors.
P_{HB}	Proportion of herbivorous birds in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{HB}	Fraction of diet comprised of herbivorous birds	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of herbivorous birds. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-6

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_{OM}	Concentration of COPC in omnivorous mammals	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-5)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-5. Uncertainties associated with this variable include: (1) Variables *Cs* and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables will be site-specific. (2) Variables $BCF_{S\text{-}OM}$ and $BCF_{W\text{-}OM}$ are based on biotransfer factors for beef (Ba_{beef}), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific omnivorous mammals.
P_{OM}	Proportion of omnivorous mammal diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{OM}	Fraction of diet comprised of omnivorous mammals	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of omnivorous mammals. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-6

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_{HM}	Concentration of COPC in herbivorous mammals	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-9)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-9. Uncertainties associated with this variable include: (1) Variables *Cs* and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables will be site-specific. (2) Variables $BCF_{S\text{-}HM}$ and $BCF_{W\text{-}HM}$ are based on biotransfer factors for beef cattle (Ba_{beef}), and receptor-specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific herbivorous mammals.
P_{HM}	Proportion of herbivorous mammal in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. Uncertainties associated with this variable include: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{HM}	Fraction of diet comprised of herbivorous mammals	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of herbivorous mammals. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of herbivorous mammals depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. Therefore a default value of 100 percent for the exclusive diet, may over-estimate dietary exposure.

TABLE F-2-6

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_{OB}	Concentration of COPC in omnivorous birds	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-6)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-6. Uncertainties associated with this variable include: (1) Variables *Cs* and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables will be site-specific. (2) Variables $BCF_{S\text{-}OB}$ and $BCF_{W\text{-}OB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific omnivorous birds.
P_{OB}	Proportion of omnivorous bird diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{OB}	Fraction of diet comprised of omnivorous birds	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of omnivorous birds. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-6

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
Cs	COPC concentration in soil	mg COPC /kg DW soil	**Varies** This variable is COPC- and site-specific, and should be calculated using the equation in Table B-1-1. *Cs* is expressed on a dry weight basis. Uncertainties associated with this variable include: (1) For soluble COPCs, leaching might lead to movement to below 1 centimeter in untilled soils, resulting a greater mixing depth. This uncertainty may overestimate *Cs*. (2) Deposition to hard surfaces may result in dust residues that have negligible dilution (as a result of potential mixing with *in situ* materials) in comparison to that of other residues. This uncertainty may underestimate *Cs* (3) Modeled soil concentrations may not accurately represent site-specific conditions. As a result, the actual COPC concentration in soil may be under- or overestimated to an unknown degree.
$IR_{S\text{-}CB}$	Soil ingestion rate for carnivorous bird	kg DW/kg BW-day	**Varies** This variable is site-, receptor-, and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. Uncertainties associated with this variable include the following: (1) IR_S values may under- or over-estimate BCF_S when applied for site-specific organisms.
P_S	Proportion of ingested soil that is contamanted	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-2-6

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values. The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wctot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, the uncertainty associated with using default *OC* values may be significant in specific cases.
$IR_{W\text{-}CB}$	Water ingestion rate for carnivorous bird	L/kg DW-day	**Varies** This variable is receptor- and habitat-specific, and is discussed in Chapter 5.. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. The following uncertainty is associated with this variable: (1) Water ingestion rates are strongly influenced by animal behavior and environmental factors and may over- or under- estimate $BCF_{W\text{-}CB}$ to an unknown degree.
P_W	Proportion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

TABLE F-2-6

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN FOREST, SHORTGRASS PRAIRIE, TALLGRASS PRAIRIE, AND SHRUB/SCRUB FOOD WEBS

REFERENCES AND DISCUSSIONS

U.S. EPA. 1993. *Wildlife Exposure Factor Handbook.* Volumes I and II. Office of Research and Development. EPA/600/R-93/187a

TABLE F-2-7

COPC DOSE INGESTED TERMS IN HERBIVOROUS MAMMALS IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Description

This equation calculates the daily dose through the ingestion of contaminated food/prey, sediment, and water in aquatic herbivorous mammals in freshwater marsh, brackish/intermediate marsh, and saltwater marsh food webs. The limitations and uncertainties introduced in calculating this variable include the following:

(1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables will be site-specific.
(2) Variables $BCF_{BS\text{-}HM}$, and $BCF_{W\text{-}HM}$ are based on biotransfer factors for beef cattle (Ba_{beef}), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute a representative daily dose for site-specific herbivorous mammals.

Equation

$$D_{HM} = \left(C_{AV} \cdot IR_{HM} \cdot P_{AV} \cdot F_{AV}\right) + \left(C_{AL} \cdot IR_{HM} \cdot P_{AL} \cdot F_{AL}\right) + \left(C_{sed} \cdot IR_{S\text{-}HM} \cdot P_S\right) + \left(C_{wctot} \cdot IR_{W\text{-}HM} \cdot P_W\right)$$

Variable	Description	Units	Value
D_{HM}	Dose COPC ingested for aquatic herbivorous mammals	mg COPC/kg BW-day	
C_{AV}	Concentration of COPC in aquatic vegetation	mg COPC/kg WW	**Varies (calculated - Table F-1-7)** This variable is site- and COPC-specific; it is calculated using the equation in Table F-1-7. Uncertainties associated with this variable include: (1) C_{sed} values are COPC- and site-specific. Uncertainties associated with this variable will be site-specific. (2) $BCF_{S\text{-}AV}$ values are intended to represent "generic aquatic vegetation species", and therefore may over- or under-estimate exposure when applied to site-specific vegetation.

TABLE F-2-7

COPC DOSE INGESTED TERMS IN HERBIVOROUS MAMMALS IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
IR_{HM}	Food ingestion rate of aquatic herbivorous mammal	kg WW/kg BW-day	**Varies** This variable is receptor-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are provided in Chapter 5, Table 5-1. Uncertainties associated with this variable include: (1) Food ingestion rates are influenced by several factors including: metabolic rate, energy requirements for growth and reproduction, and dietary composition. Ingestion rates are also influenced by ambient temperature, receptor activity level and body weight U.S. EPA (1993). These factors introduce an unknown degree of uncertainty when used to estimate daily dose. (2) *IR* values may over- or under- estimate exposure when applied for site-specific receptors.
P_{AV}	Proportion of aquatic vegetation in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{AV}	Fraction of diet comprised of aquatic vegetation	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic vegetation. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-7

COPC DOSE INGESTED TERMS IN HERBIVOROUS MAMMALS IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{AL}	Concentration of COPC in algae	mg COPC/kg WW	**Varies (calculated - Table F-1-8)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-8. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. Uncertainties associated with this variable will be site-specific. (2) $BCF_{W\text{-}AL}$ values are intended to represent "generic algae species", and therefore may over- or under-estimate exposure when applied to site-specific species.
P_{AL}	Proportion of algae in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{AL}	Fraction of diet comprised of algae	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of algae. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-7

COPC DOSE INGESTED TERMS IN HERBIVOROUS MAMMALS IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{sed}	COPC concentration in bed sediment	mg COPC/kg DW sediment	**Varies (calculated - Table B-2-19)** This equation calculates the concentration of COPCs in bed sediments. Uncertainties associated with this equation include the following: (1) The default variable values recommended for use in the equation in Table B-2-19 may not accurately represent site-specific water body conditions. The degree of uncertainty associated with default variable values is expected to be limited either because the probable ranges for these variables are narrow or because information allowing reasonable estimates is generally available. (2) Uncertainties associated with variables f_{bs}, C_{wctot} and Kd_{bs} are largely associated with the use of default *OC* content values in their calculation. The uncertainty may be significant in specific instances, because *OC* content is known to vary widely in different locations in the same medium. This variable is site-specific.
$IR_{S\text{-}HM}$	Sediment ingestion rate for aquatic herbivorous mammal	kg DW/kg BW-day	**Varies** This variable is site-, receptor-, and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. Uncertainties associated with this variable include the following: (1) IR_S values may under- or over-estimate BCF_S when applied for site-specific organisms.
P_S	Proportion of ingested bed sediment that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of sediment ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-2-7

COPC DOSE INGESTED TERMS IN HERBIVOROUS MAMMALS IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values. Uncertainties may also be associated with the variable L_T and k_{wt}. The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wctot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, the uncertainty associated with using default *OC* values may be significant in specific cases.
$IR_{W\text{-}HM}$	Water ingestion rate for aquatic herbivorous mammal	L/kg-BW-day	**Varies** This variable is receptor- and habitat-specific, and is discussed in Chapter 5.. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. The following uncertainty is associated with this variable: (1) Water ingestion rates are influenced by animal behavior and environmental factors and may over- or under-estimate $BCF_{W\text{-}HM}$ to an unknown degree.
P_W	Proportion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

TABLE F-2-7

COPC DOSE INGESTED TERMS IN HERBIVOROUS MAMMALS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

REFERENCES AND DISCUSSIONS

U.S. EPA. 1993. *Wildlife Exposure Factor Handbood.* Volumes I and II. Office of Research and Development. EPA/600/R-93/187a

TABLE F-2-8

COPC DOSE INGESTED TERMS IN HERBIVOROUS BIRDS IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Description

This equation calculates the daily dose through ingestion of contaminated food/prey, sediment, and water in aquatic herbivorous birds in freshwater marsh, brackish/intermediate marsh, and saltwater marsh food webs. The limitations and uncertainties introduced in calculating this variable include the following:

(1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables will be site-specific.
(2) Variables $BCF_{S\text{-}HB}$ and $BCF_{W\text{-}HB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor-specific ingestion rates, and therefore may introduce uncertainty when used to compute a representative daily dose for site-specific herbivorous birds.

Equation

$$D_{HB} = \left(C_{AV} \cdot IR_{HB} \cdot P_{AV} \cdot F_{AV}\right) + \left(C_{AL} \cdot IR_{HB} \cdot P_{AL} \cdot F_{AL}\right) + \left(C_{sed} \cdot IR_{S\text{-}HB} \cdot P_S\right) + \left(C_{wctot} \cdot IR_{W\text{-}HB} \cdot P_W\right)$$

Variable	Description	Units	Value
D_{HB}	Dose ingested for herbivorous birds	mg/kg BW-day	
C_{AV}	Concentration of COPC in aquatic vegetation	mg COPC/kg WW	**Varies (calculated - Table F-1-7)** This variable is site- and COPC-specific; it is calculated using the equation in Table F-1-7. Uncertainties associated with this variable include: (1) C_{sed} values are COPC- and site-specific. (2) $BCF_{S\text{-}AV}$ values are intended to represent "generic aquatic vegetation species", and therefore may over- or under-estimate exposure when applied to site-specific vegetation.
IR_{HB}	Food ingestion rate of aquatic herbivorous bird	kg WW/kg BW-day	**Varies** This variable is receptor-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are provided in Chapter 5, Table 5-1. Uncertainties associated with this variable include: (1) Food ingestion rates are influenced by several factors including: metabolic rate, energy requirements for growth and reproduction, and dietary composition. Ingestion rates are also influenced by ambient temperature, receptor activity level and body weight U.S. EPA (1993). These factors introduce an unknown degree of uncertainty when used to estimate daily dose. (2) IR values may over- or under- estimate exposure when applied for site-specific receptors.

TABLE F-2-8

COPC DOSE INGESTED TERMS IN HERBIVOROUS BIRDS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
P_{AV}	Proportion of aquatic vegetation in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{AV}	Fraction of diet comprised of aquatic vegetation	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic vegetation. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.
C_{AL}	Concentration of COPC in algae	mg COPC/kg WW	**Varies (calculated - Table F-1-8)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-8. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. Uncertainties associated with this variable will be site-specific. (2) $BCF_{W\text{-}AL}$ values are intended to represent "generic algae species", and therefore may over- or under-estimate exposure when applied to site-specific species.

TABLE F-2-8

COPC DOSE INGESTED TERMS IN HERBIVOROUS BIRDS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

(Page 3 of 6)

Variable	Description	Units	Value
P_{AL}	Proportion of algae in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{AL}	Fraction of diet comprised of algae	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of algae. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-8

COPC DOSE INGESTED TERMS IN HERBIVOROUS BIRDS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{sed}	COPC concentration in bed sediment	mg COPC/kg DW sediment	**Varies (calculated - Table B-2-19)** This equation calculates the concentration of COPCs in bed sediments. Uncertainties associated with this equation include the following: (1) The default variable values recommended for use in the equation in Table B-2-19 may not accurately represent site-specific water body conditions. The degree of uncertainty associated with default variable values is expected to be limited either because the probable ranges for these variables are narrow or because information allowing reasonable estimates is generally available. (2) Uncertainties associated with variables f_{bs}, C_{wctot} and Kd_{bs} are largely associated with the use of default *OC* content values in their calculation. The uncertainty may be significant in specific instances, because *OC* content is known to vary widely in different locations in the same medium. This variable is site-specific.
$IR_{S\text{-}HB}$	Sediment ingestion rate for herbivorous bird	kg DW/kg BW-day	**Varies** This variable is site-, receptor-, and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. Uncertainties associated with this variable include the following: (1) IR_S values may under- or over-estimate BCF_S when applied for site-specific organisms.
P_S	Proportion of ingested bed sediment that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-2-8

COPC DOSE INGESTED TERMS IN HERBIVOROUS BIRDS IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

(Page 5 of 6)

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values. Uncertainties may also be associated with the variable L_T and k_{wt}. The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wctot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, the uncertainty associated with using default *OC* values may be significant in specific cases.
$IR_{W\text{-}HB}$	Water ingestion rate for aquatic herbivorous bird	L/kg BW-day	**Varies** This variable is receptor- and habitat-specific, and is discussed in Chapter 5, Section 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. The following uncertainty is associated with this variable: (1) Water ingestion rates are influenced by animal behavior and environmental factors and may over- or under-estimate $BCF_{W\text{-}HB}$ to an unknown degree.
P_W	Proportion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

TABLE F-2-8

COPC DOSE INGESTED TERMS IN HERBIVOROUS BIRDS
IN FRESHWATER/WETLAND, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

REFERENCES AND DISCUSSIONS

U.S. EPA. 1993. *Wildlife Exposure Factor Handbook.* Volumes I and II. Office of Research and Development. EPA/600/R-93/187a

TABLE F-2-9

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS IN FRESHWATER/WETLAND MARSH, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Description

This equation calculates the daily dose through ingestion of contaminated food/prey, sediment, and water in aquatic omnivorous mammals in freshwater marsh, brackish/intermediate marsh, and saltwater marsh food webs. The limitations and uncertainties introduced in calculating this variable include the following:

(1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables will be site-specific .
(2) Variables $BCF_{S\text{-}OM}$ and $BCF_{W\text{-}OM}$ are based on biotransfer factors for beef cattle (Ba_{beef}), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute a representative daily dose for site-specific omnivorous mammals.

Equation

$$D_{OM} = \left(C_{HM} \cdot IR_{OM} \cdot P_{HM} \cdot F_{HM}\right) + \left(C_{HB} \cdot IR_{OM} \cdot P_{HB} \cdot F_{HB}\right) + \left(C_{BI} \cdot IR_{OM} \cdot P_{BI} \cdot F_{BI}\right) + \left(C_{WI} \cdot IR_{OM} \cdot P_{WI} \cdot F_{WI}\right)$$
$$+ \left(C_{AV} \cdot IR_{OM} \cdot P_{AV} \cdot F_{AV}\right) + \left(C_{AL} \cdot IR_{OM} \cdot P_{AL} \cdot F_{AL}\right) + \left(C_{sed} \cdot IR_{S\text{-}OM} \cdot P_{S}\right) + \left(C_{wctot} \cdot IR_{W\text{-}OM} \cdot P_{W}\right)$$

Variable	Description	Units	Value
D_{OM}	Dose ingested for omnivorous mammals	mg/kg BW-day	
C_{HM}	Concentration of COPC in aquatic herbivorous mammals	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-9)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-9. Uncertainties associated with this variable include: (1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. (2) Variables $BCF_{S\text{-}HM}$ and $BCF_{W\text{-}HM}$ are based on biotransfer factors for beef cattle (Ba_{beef}), and receptor-specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific omnivorous mammals.

TABLE F-2-9

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS
IN FRESHWATER/WETLAND MARSH, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
IR_{OM}	Food ingestion rate of aquatic omnivorous mammal	kg WW/kg BW-day	**Varies** This variable is receptor-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are provided in Chapter 5, Table 5-1. Uncertainties associated with this variable include: (1) Food ingestion rates are influenced by several factors including: metabolic rate, energy requirements for growth and reproduction, and dietary composition. Ingestion rates are also influenced by ambient temperature, receptor activity level and body weight U.S. EPA (1993). These factors introduce an unknown degree of uncertainty when used to estimate daily dose. (2) IR values may over- or under- estimate exposure when applied for site-specific receptors.
P_{HM}	Proportion of aquatic herbivorous mammal in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{HM}	Fraction of diet comprised of aquatic herbivorous mammals	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic herbivorous mammals. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-9

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS IN FRESHWATER/WETLAND MARSH, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{HB}	Concentration of COPC in aquatic herbivorous birds	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-10)** This variable is site-specific and COPC-specific, and is calculated using the equation in Table F-1-10. Uncertainties associated with this variable include: (1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. (2) Variables $BCF_{S\text{-}HB}$ and $BCF_{W\text{-}HB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific aquatic herbivorous birds.
P_{HB}	Proportion of aquatic herbivorous birds in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{HB}	Fraction of diet comprised of aquatic herbivorous birds	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic herbivorous birds. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-9

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS
IN FRESHWATER/WETLAND MARSH, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{BI}	Concentration of COPC in benthic invertebrates	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-11)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-11. Uncertainties associated with this variable include the following: (1) C_{sed} values are COPC- and site-specific. Uncertainties associated with this variable will be site-specific. (2) $BCF_{S\text{-}BI}$ values are intended to represent "generic benthic invertebrate species", and therefore may over- or under-estimate exposure when applied to site-specific organisms.
P_{BI}	Proportion of benthic invertebrate in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{BI}	Fraction of diet comprised of benthic invertebrates	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of benthic invertebrates. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-9

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS
IN FRESHWATER/WETLAND MARSH, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{WI}	Concentration of COPC in water invertebrates	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-12)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-12. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. (2) $BCF_{W\text{-}WI}$ values are intended to represent "generic water invertebrate species", and therefore may over- or under-estimate exposure when applied to site-specific organisms.
P_{WI}	Proportion of water invertebrate in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{WI}	Fraction of diet comprised of water invertebrates	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of water invertebrates. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-9

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS IN FRESHWATER/WETLAND MARSH, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{AV}	Concentration of COPC in aquatic vegetation	mg COPC/kg WW	**Varies (calculated - Table F-1-7)** This variable is site- and COPC-specific; it is calculated using the equation in Table F-1-7. Uncertainties associated with this variable include: (1) C_{sed} values are COPC- and site-specific. (2) $BCF_{S\text{-}AV}$ values are intended to represent "generic aquatic vegetation species", and therefore may over- or under-estimate exposure when applied to site-specific vegetation.
P_{AV}	Proportion of aquatic vegetation in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{AV}	Fraction of diet comprised of aquatic vegetation	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic vegetation. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-9

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS IN FRESHWATER/WETLAND MARSH, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{AL}	Concentration of COPC in algae	mg COPC/kg WW	**Varies (calculated - Table F-1-8)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-8. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. (2) $BCF_{W\text{-}AL}$ values are intended to represent "generic algae species", and therefore may over- or under-estimate exposure when applied to site-specific species.
P_{AL}	Proportion of algae in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{AL}	Fraction of diet comprised of algae	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of algae. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-9

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS
IN FRESHWATER/WETLAND MARSH, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

Variable	Description	Units	Value
C_{sed}	COPC concentration in bed sediment	mg COPC/kg DW sediment	**Varies (calculated - Table B-2-19)** This equation calculates the concentration of contaminants sorbed to bed sediments. Uncertainties associated with this equation include the following: (1) The default variable values recommended for use in the equation in Table B-2-19 may not accurately represent site-specific water body conditions. The degree of uncertainty associated with default variable values is expected to be limited either because the probable ranges for these variables are narrow or because information allowing reasonable estimates is generally available. (2) Uncertainties associated with variables f_{bs}, C_{wctot} and Kd_{bs} are largely associated with the use of default *OC* content values in their calculation. The uncertainty may be significant in specific instances, because *OC* content is known to vary widely in different locations in the same media. This variable is site-specific.
$IR_{S\text{-}OM}$	Sediment ingestion rate for aquatic omnivorous mammal	kg DW/kg BW-day	**Varies** This variable is site-, receptor-, and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. Uncertainties associated with this variable include the following: (1) IR_S values may under- or over-estimate BCF_S when applied to site-specific organisms.
P_S	Portion of ingested bed sediment that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-2-9

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS
IN FRESHWATER/WETLAND MARSH, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

(Page 9 of 10)

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values. Uncertainties may also be associated with the variable L_T and k_{wt} The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wctot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same media, the uncertainty associated with using default *OC* values may be significant in specific cases.
$IR_{W\text{-}OM}$	Water ingestion rate for aquatic omnivorous mammal	L/kg BW-day	**Varies** This variable is receptor- and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. The following uncertainty is associated with this variable: (1) Water ingestion rates are strongly influenced by animal behavior and environmental factors and may over- or under- estimate $BCF_{W\text{-}OM}$ to an unknown degree.
P_W	Portion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

TABLE F-2-9

COPC DOSE INGESTED TERMS IN OMNIVOROUS MAMMALS
IN FRESHWATER/WETLAND MARSH, BRACKISH/INTERMEDIATE MARSH, AND SALTMARSH FOOD WEBS

REFERENCES AND DISCUSSIONS

U.S. EPA. 1993. *Wildlife Exposure Factor Handbood.* Volumes I and II. Office of Research and Development. EPA/600/R-93/187a

TABLE F-2-10

COPC DOSE INGESTED TERMS IN OMNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Description

This equation calculates the daily dose through ingestion of contaminated food/prey, sediment, and water in aquatic omnivorous birds in freshwater marsh, brackish/intermediate marsh, and saltwater marsh food webs. The limitations and uncertainties introduced in calculating this variable include the following:

(1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables will be site-specific .
(2) Variables $BCF_{S\text{-}OB}$ and $BCF_{W\text{-}OB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute a representative daily dose for site-specific omnivorous birds.

Equation

$$D_{OB} = \left(C_{BI} \cdot IR_{OB} \cdot P_{BI} \cdot F_{BI}\right) + \left(C_{WI} \cdot IR_{OB} \cdot P_{WI} \cdot F_{WI}\right) + \left(C_{AV} \cdot IR_{OB} \cdot P_{AV} \cdot F_{AV}\right)$$
$$+ \left(C_{AL} \cdot IR_{OB} \cdot P_{AL} \cdot F_{AL}\right) + \left(C_{sed} \cdot IR_{S\text{-}OB} \cdot P_{S}\right) + \left(C_{wctot} \cdot IR_{W\text{-}OB} \cdot P_{W}\right)$$

Variable	Description	Units	Value
D_{OB}	Dose ingested for aquatic omnivorous birds	mg/kg BW-day	
C_{BI}	Concentration of COPC in benthic invertebrates	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-11)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-11. Uncertainties associated with this variable include the following: (1) C_{sed} values are COPC- and site-specific. (2) $BCF_{S\text{-}BI}$ values are intended to represent "generic benthic invertebrate species", and therefore may over- or under-estimate exposure when applied to site-specific organisms.

TABLE F-2-10

COPC DOSE INGESTED TERMS IN OMNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
IR_{OB}	Food ingestion rate of aquatic omnivorous bird	kg WW/kg BW-day	**Varies** This variable is receptor-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are provided in Chapter 5, Table 5-1. Uncertainties associated with this variable include: (1) Food ingestion rates are influenced by several factors including: metabolic rate, energy requirements for growth and reproduction, and dietary composition. Ingestion rates are also influenced by ambient temperature, receptor activity level and body weight U.S. EPA (1993). These factors introduce an unknown degree of uncertainty when used to estimate daily dose. (2) IR values may over- or under- estimate exposure when applied for site-specific receptors.
P_{BI}	Proportion of benthic invertebrate in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{BI}	Fraction of diet comprised of benthic invertebrates	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of benthic invertebrates. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-10

COPC DOSE INGESTED TERMS IN OMNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{WI}	Concentration of COPC in water invertebrates	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-12)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-12. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. (2) $BCF_{W\text{-}WI}$ values are intended to represent "generic water invertebrate species", and therefore may over- or under-estimate exposure when applied to site-specific organisms.
P_{WI}	Proportion of water invertebrate in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{WI}	Fraction of diet comprised of water invertebrates	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of water invertebrates. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-10

COPC DOSE INGESTED TERMS IN OMNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{AV}	Concentration of COPC in aquatic vegetation ingested by the animal	mg COPC/kg WW	**Varies (calculated - Table F-1-7)** This variable is site- and COPC-specific; it is calculated using the equation in Table F-1-7. Uncertainties associated with this variable include: (1) C_{sed} values are COPC- and site-specific. (2) $BCF_{S\text{-}AV}$ values are intended to represent "generic aquatic vegetation species", and therefore may over- or under-estimate exposure when applied to site-specific vegetation.
P_{AV}	Proportion of aquatic vegetation in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{AV}	Fraction of diet comprised of aquatic vegetation	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic vegetation. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-10

COPC DOSE INGESTED TERMS IN OMNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{sed}	COPC concentration in bed sediment	mg COPC/kg DW sediment	**Varies (calculated - Table B-2-19)** This equation calculates the concentration of COPCs in bed sediments. Uncertainties associated with this equation include the following: (1) The default variable values recommended for use in the equation in Table B-2-19 may not accurately represent site-specific water body conditions. The degree of uncertainty associated with default variable values is expected to be limited either because the probable ranges for these variables are narrow or because information allowing reasonable estimates is generally available. (2) Uncertainties associated with variables f_{bs}, C_{wctot} and Kd_{bs} are largely associated with the use of default *OC* content values in their calculation. The uncertainty may be significant in specific instances, because *OC* content is known to vary widely in different locations in the same medium. This variable is site-specific.
IR_{SOB}	Sediment ingestion rate for aquatic omnivorous bird	kg DW/kg BW-day	**Varies** This variable is site-, receptor-, and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. Uncertainties associated with this variable include the following: (1) IR_S values may under- or over-estimate BCF_S when applied to site-specific organisms.
P_S	Portion of ingested bed sediment that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-2-10

COPC DOSE INGESTED TERMS IN OMNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values. Uncertainties may also be associated with the variable L_T and k_{wt}. The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wtot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same media, the uncertainty associated with using default *OC* values may be significant in specific cases.
$I_{W\text{-}OB}$	Water ingestion rate for aquatic omnivorous bird	L/kg BW-day	**Varies** This variable is receptor- and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. The following uncertainty is associated with this variable: (1) Water ingestion rates are influenced by animal behavior and environmental factors and may over- or under-estimate $BCF_{W\text{-}HM}$ to an unknown degree.
P	Portion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated may be overestimated.

TABLE F-2-10

COPC DOSE INGESTED TERMS IN OMNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

REFERENCES AND DISCUSSIONS

U.S. EPA. 1993. *Wildlife Exposure Factor Handbook.* Volumes I and II. Office of Research and Development. EPA/600/R-93/187a.

TABLE F-2-11

EQUATIONS FOR COMPUTING COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Description

This equation calculates the daily dose through exposure to food/prey, sediment, and water in aquatic carnivorous mammals in freshwater marsh, brackish/intermediate marsh, and saltwater marsh food webs. The limitations and uncertainties introduced in calculating this variable include the following:

(1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables will be site-specific
(2) Variables $BCF_{S\text{-}CM}$, and $BCF_{W\text{-}CM}$ are based on biotransfer factors for beef cattle (Ba_{beef}), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute a representative daily dose for site-specific carnivorous mammals.

Equation

$$D_{CM} = \left(C_{HB} \cdot IR_{CM} \cdot P_{HB} \cdot F_{HB}\right) + \left(C_{OF} \cdot IR_{CM} \cdot P_{OF} \cdot F_{OF}\right) + \left(C_{CF} \cdot IR_{CM} \cdot P_{CF} \cdot F_{CF}\right) + \left(C_{OB} \cdot IR_{CM} \cdot P_{OB} \cdot F_{OB}\right)$$
$$+ \left(C_{OM} \cdot IR_{CM} \cdot P_{OM} \cdot F_{OM}\right) + \left(C_{HM} \cdot IR_{CM} \cdot P_{HM} \cdot F_{HM}\right) + \left(C_{sed} \cdot IR_{S\text{-}CM} \cdot P_{S}\right) + \left(C_{wctot} \cdot IR_{W\text{-}CM} \cdot P_{W}\right)$$

Variable	Description	Units	Value
D_{CM}	Dose ingested for carnivorous mammals	mg/kg BW-day	
C_{HB}	Concentration of COPC in herbivorous birds	mg COPC/kg FW tissue	**Varies** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-10. Uncertainties associated with this variable include: (1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. (2) Variables $BCF_{S\text{-}HB}$ and $BCF_{W\text{-}HB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific herbivorous birds.

TABLE F-2-11

EQUATIONS FOR COMPUTING COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
IR_{CM}	Food ingestion rate of carnivorous mammal	kg WW/kg BW-day	**Varies** This variable is receptor-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are provided in Chapter 5, Table 5-1. Uncertainties associated with this variable include: (1) Food ingestion rates are influenced by several factors including: metabolic rate, energy requirements for growth and reproduction, and dietary composition. Ingestion rates are also influenced by ambient temperature, receptor activity level and body weight U.S. EPA (1993). These factors introduce an unknown degree of uncertainty when used to estimate daily dose. (2) IR values may over- or under- estimate exposure when applied for site-specific receptors.
P_{HB}	Proportion of herbivorous birds in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{HB}	Fraction of diet comprised of herbivorous birds	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic herbivorous birds. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-11

EQUATIONS FOR COMPUTING COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{OF}	Concentration of COPC in omnivorous fish	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-16)** This variable is site-specific and COPC-specific; it is calculated using the equation in F-1-16. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. (2) The data set used to calculate BCF_{fish} is based on a limited number of test organisms and therefore may over- or under-estimate exposure when applied for site-specific organisms.
P_{OF}	Proportion of omnivorous fish diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{OF}	Fraction of diet comprised of omnivorous fish	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of omnivorous fish. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-11

EQUATIONS FOR COMPUTING COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{CF}	Concentration in carnivorous fish	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-17)** This variable is site-specific and COPC-specific; it is calculated using the equation in F-1-17. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. (2) The data set used to calculate BCF_{fish} is based on a limited number of test organisms and therefore may over- or under-estimate exposure when applied to site-specific organisms.
P_{CF}	Proportion of carnivorous fish in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{CF}	Fraction of diet comprised of carnivorous fish	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of carnivorous fish. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-11

EQUATIONS FOR COMPUTING COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{OB}	Concentration of COPC in omnivorous birds	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-15)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-6. Uncertainties associated with this variable include: (1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. (2) Variables $BCF_{S\text{-}OB}$ and $BCF_{W\text{-}OB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific aquatic omnivorous birds.
P_{OB}	Proportion of omnivorous bird diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{OB}	Fraction of diet comprised of omnivorous birds	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic omnivorous birds. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-11

EQUATIONS FOR COMPUTING COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{OM}	Concentration of COPC in omnivorous mammals	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-5)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-5. Uncertainties associated with this variable include: (1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. (2) Variables $BCF_{S\text{-}OM}$ and $BCF_{W\text{-}OM}$ are based on biotransfer factors for beef (Ba_{beef}), and receptor-specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific omnivorous mammals.
P_{OM}	Proportion of omnivorous mammal diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{OM}	Fraction of diet comprised of omnivorous mammals	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of omnivorous mammals. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-11

EQUATIONS FOR COMPUTING COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{HM}	Concentration of COPC in herbivorous mammals	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-9)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-9. Uncertainties associated with this variable include: (1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. (2) Variables $BCF_{S\text{-}HM}$ and $BCF_{W\text{-}HM}$ are based on biotransfer factors for beef cattle (Ba_{beef}), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific aquatic herbivorous mammals.
P_{HM}	Proportion of herbivorous mammal in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. Uncertainties associated with this variable include: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{HM}	Fraction of diet comprised of herbivorous mammals	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic herbivorous mammals. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of herbivorous mammals depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. Therefore a default value of 100 percent for the exclusive diet, may over-estimate dietary exposure.

TABLE F-2-11

EQUATIONS FOR COMPUTING COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{sed}	COPC concentration in bed sediment	mg COPC/kg DW sediment	**Varies (calculated - Table B-2-19)** This equation calculates the concentration of contaminants sorbed to bed sediments. Uncertainties associated with this equation include the following: (1) The default variable values recommended for use in the equation in Table B-2-19 may not accurately represent site-specific water body conditions. The degree of uncertainty associated with default variable values is expected to be limited either because the probable ranges for these variables are narrow or because information allowing reasonable estimates is generally available. (2) Uncertainties associated with variables f_{bs}, C_{wctot} and Kd_{bs} are largely associated with the use of default *OC* content values in their calculation. The uncertainty may be significant in specific instances, because *OC* content is known to vary widely in different locations in the same medium. This variable is site-specific.
$IR_{S\text{-}CM}$	Sediment ingestion rate for carnivorous mammal	kg DW/kg BW-day	**Varies** This variable is site-, receptor-, and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. Uncertainties associated with this variable include the following: (1) IR_S values may under- or over-estimate BCF_S when applied to site-specific organisms.
P_S	Portion of ingested bed sediment that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-2-11

EQUATIONS FOR COMPUTING COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values. Uncertainties may also be associated with the variable L_T and k_{wt}. The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wctot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, the uncertainty associated with using default *OC* values may be significant in specific cases.
$IR_{W\text{-}CM}$	Water ingestion rate for carnivorous mammal	kg WW/kg BW-day	**Varies** This variable is receptor- and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. The following uncertainty is associated with this variable: (1) Water ingestion rates are strongly influenced by animal behavior and environmental factors and may over- or under- estimate $BCF_{W\text{-}HM}$ to an unknown degree.
P_W	Portion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW rsecommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

TABLE F-2-11

EQUATIONS FOR COMPUTING COPC DOSE INGESTED TERMS IN CARNIVOROUS MAMMALS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

(Page 10 of 10)

REFERENCES AND DISCUSSION

U.S. EPA. 1993. *Wildlife Exposure Factor Handbood.* Volumes I and II. Office of Research and Development. EPA/600/R-93/187a

TABLE F-2-12

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Description

This equation calculates the daily dose through exposure to contaminated food/prey, soil, and water in aquatic carnivorous birds in freshwater marsh, brackish/intermediate marsh, and saltwater marsh food webs. The limitations and uncertainties introduced in calculating this variable include the following:

(1) Variables C_{sed}, and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables will be site-specific.
(2) Variables $BCF_{BS\text{-}CB}$, and $BCF_{W\text{-}CB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute a representative daily dose for site-specific carnivorous birds.

Equation

$$D_{CB} = \left(C_{OF} \cdot IR_{CB} \cdot P_{OF} \cdot F_{OF}\right) + \left(C_{CF} \cdot IR_{CB} \cdot P_{CF} \cdot F_{CF}\right) + \left(C_{OM} \cdot IR_{CB} \cdot P_{OM} \cdot F_{OM}\right) + \left(C_{HM} \cdot IR_{CB} \cdot P_{HM} \cdot F_{HM}\right)$$
$$+ \left(C_{OB} \cdot IR_{CB} \cdot P_{OB} \cdot F_{OB}\right) + \left(C_{HB} \cdot IR_{CB} \cdot P_{HB} \cdot F_{HB}\right) + \left(C_{sed} \cdot IR_{S\text{-}CB} \cdot P_{S}\right) + \left(C_{wctot} \cdot IR_{W\text{-}CB} \cdot P_{W}\right)$$

Variable	Description	Units	Value
D_{CB}	Dose ingested for carnivorous birds	mg/kg BW-day	
C_{OF}	Concentration of COPC in omnivorous fish	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-16)** This variable is site-specific and COPC-specific; it is calculated using the equation in F-1-16. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. (2) The data set used to calculate BCF_{fish} is based on a limited number of test organisms and therefore may over- or under-estimate exposure when applied to site-specific organisms.

TABLE F-2-12

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
IR_{CB}	Food ingestion rate of carnivorous birds	kg WW/kg BW-day	**Varies** This variable is receptor-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are provided in Chapter 5, Table 5-1. Uncertainties associated with this variable include: (1) Food ingestion rates are influenced by several factors including: metabolic rate, energy requirements for growth and reproduction, and dietary composition. Ingestion rates are also influenced by ambient temperature, receptor activity level and body weight U.S. EPA (1993). These factors introduce an unknown degree of uncertainty when used to estimate daily dose. (2) *IR* values may over- or under- estimate exposure when applied to site-specific receptors.
P_{OF}	Proportion of omnivorous fish diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{OF}	Fraction of diet comprised of omnivorous fish	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of omnivorous fish. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-12

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

(Page 3 of 11)

Variable	Description	Units	Value
C_{CF}	Concentration in carnivorous fish	mg COPC/kg FW tissue	**Varies** This variable is site-specific and COPC-specific; it is calculated using the equation in F-1-17. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. (2) The data set used to calculate BCF_{fish} is based on a limited number of test organisms and therefore may over- or under-estimate exposure when applied to site-specific organisms.
P_{CF}	Proportion of carnivorous fish diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{CF}	Fraction of diet comprised of carnivorous fish	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of carnivorous fish. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-12

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{OM}	Concentration of COPC in omnivorous mammals	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-5)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-5. Uncertainties associated with this variable include: (1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. (2) Variables $BCF_{S\text{-}OM}$ and $BCF_{W\text{-}OM}$ are based on biotransfer factors for beef (Ba_{beef}), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific aquatic omnivorous mammals.
P_{OM}	Proportion of aquatic omnivorous mammal in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{OM}	Fraction of diet comprised of omnivorous mammals	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic omnivorous mammals. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-12

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{HM}	Concentration of COPC in herbivorous mammals	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-9)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-9. Uncertainties associated with this variable include: (1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. (2) Variables $BCF_{S\text{-}HM}$ and $BCF_{W\text{-}HM}$ are based on biotransfer factors for beef cattle (Ba_{beef}), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific aquatic herbivorous mammals.
P_{HM}	Proportion of aquatic herbivorous mammal in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. Uncertainties associated with this variable include: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{HM}	Fraction of diet comprised of herbivorous mammals	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic herbivorous mammals. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of herbivorous mammals depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. Therefore a default value of 100 percent for the exclusive diet, may over-estimate dietary exposure.

TABLE F-2-12

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{OB}	Concentration of COPC in omnivorous birds	mg COPC/kg FW tissue	**Varies** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-6. Uncertainties associated with this variable include: (1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. (2) Variables $BCF_{S\text{-}OB}$ and $BCF_{W\text{-}OB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific aquatic omnivorous birds.
P_{OB}	Proportion of omnivorous bird in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{OB}	Fraction of diet comprised of omnivorous birds	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic omnivorous birds. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-12

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{HB}	Concentration of COPC in herbivorous birds	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-10)** This variable is site-specific and chemical-specific; it is calculated using the equation in Table F-1-10. Uncertainties associated with this variable include: (1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. (2) Variables $BCF_{S\text{-}HB}$ and $BCF_{W\text{-}HB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor-specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific aquatic herbivorous birds.
P_{HB}	Proportion of herbivorous birds in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{HB}	Fraction of diet comprised of herbivorous birds	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of aquatic herbivorous birds. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-12

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{sed}	COPC concentration in bed sediment	mg COPC/kg DW sediment	**Varies (calculated - Table B-2-19)** This equation calculates the concentration of COPCs in bed sediments. Uncertainties associated with this equation include the following: (1) The default variable values recommended for use in the equation in Table B-2-19 may not accurately represent site-specific water body conditions. The degree of uncertainty associated with default variable values is expected to be limited either because the probable ranges for these variables are narrow or because information allowing reasonable estimates is generally available. (2) Uncertainties associated with variables f_{bs}, C_{wctot} and Kd_{bs} are largely associated with the use of default *OC* content values in their calculation. The uncertainty may be significant in specific instances, because *OC* content is known to vary widely in different locations in the same medium. This variable is site-specific.
$IR_{S\text{-}CB}$	Sediment ingestion rate for carnivorous bird	kg DW/kg BW-day	**Varies** This variable is site-, receptor-, and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. Uncertainties associated with this variable include the following: (1) IR_S values may under- or over-estimate BCF_S when applied to site-specific organisms.
P_S	Portion of ingested bed sediment that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-2-12

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values. Uncertainties may also be associated with the variable L_T and k_{wt} The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wtot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, the uncertainty associated with using default *OC* values may be significant in specific cases.
$IR_{W\text{-}CB}$	Water ingestion rate for aquatic carnivorous bird	L/kg BW-day	**Varies** This variable is receptor- and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. The following uncertainty is associated with this variable: (1) Water ingestion rates are strongly influenced by animal behavior and environmental factors and may over- or under- estimate $BCF_{W\text{-}HM}$ to an unknown degree.

TABLE F-2-12

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
P_W	Portion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

TABLE F-2-12

COPC DOSE INGESTED TERMS IN CARNIVOROUS BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

REFERENCES AND DISCUSSIONS

U.S. EPA. 1993. *Wildlife Exposure Factor Handbook.* Volumes I and II. Office of Research and Development. EPA/600/R-93/187a

TABLE F-2-13

COPC DOSE INGESTED TERMS IN CARNIVOROUS SHORE BIRDS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Description

This equation calculates the daily dose through exposure to contaminated food/prey, sediment, and water in carnivorous shore birds in freshwater marsh, brackish/intermediate marsh, and saltwater marsh food webs. The limitations and uncertainties introduced in calculating this variable include the following:

(1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. Uncertainties associated with these variables will be site-specific
(2) Variables $BCF_{S\text{-}CSB}$, and $BCF_{W\text{-}CSB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor-specific ingestion rates, and therefore may introduce uncertainty when used to compute a representative daily dose for site-specific carnivorous birds.

Equation

$$D_{CSB} = \left(C_{BI} \cdot IR_{CSB} \cdot P_{BI} \cdot F_{BI}\right) + \left(C_{WI} \cdot IR_{CSB} \cdot P_{WI} \cdot F_{WI}\right) + \left(C_{HPF} \cdot IR_{CSB} \cdot P_{HPF} \cdot F_{HPF}\right)$$
$$+ \left(C_{OF} \cdot IR_{CSB} \cdot P_{OF} \cdot F_{OF}\right) + \left(C_{OB} \cdot IR_{CSB} \cdot P_{OB} \cdot F_{OB}\right) + \left(C_{sed} \cdot IR_{S\text{-}CSB} \cdot P_{S}\right) + \left(C_{wctot} \cdot IR_{W\text{-}CSB} \cdot P_{W}\right)$$

Variable	Description	Units	Value
D_{CSB}	Dose ingested for carnivorous shore birds	mg/kg BW-day	
C_{BI}	Concentration of COPC in benthic invertebrates	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-11)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-11. Uncertainties associated with this variable include the following: (1) C_{sed} values are COPC- and site-specific. (2) $BCF_{S\text{-}BI}$ values are intended to represent "generic benthic invertebrate species", and therefore may over- or under-estimate exposure when applied to site-specific organisms.

TABLE F-2-13

COPC DOSE INGESTED TERMS IN CARNIVOROUS SHORE BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
IR_{CSB}	Food ingestion rate of carnivorous shore birds	kg WW/kg BW-day	**Varies** This variable is receptor-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are provided in Chapter 5, Table 5-1. Uncertainties associated with this variable include: (1) Food ingestion rates are influenced by several factors including: metabolic rate, energy requirements for growth and reproduction, and dietary composition. Ingestion rates are also influenced by ambient temperature, receptor activity level and body weight U.S. EPA (1993). These factors introduce an unknown degree of uncertainty when used to estimate daily dose. (2) *IR* values may over- or under- estimate exposure when applied to site-specific receptors.
P_{BI}	Proportion of benthic invertebrate in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.

TABLE F-2-13

COPC DOSE INGESTED TERMS IN CARNIVOROUS SHORE BIRDS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
F_{BI}	Fraction of diet comprised of benthic invertebrates	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of benthic invertebrates. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applided to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertaintiy and may over-estimate exposure from ingestion of a single dietary item. (3) The defalut value for an equal diet introduces uncertainity and may over- or under- estimate exposure when applied to site-specific receptors.
C_{WI}	Concentration of COPC in water invertebrates	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-12)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-12. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. (2) $BCF_{W\text{-}WI}$ values are intended to represent "generic water invertebrate species", and therefore may over- or under-estimate exposure when applied to site-specific organisms.
P_{WI}	Proportion of water invertebrate in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.

TABLE F-2-13

COPC DOSE INGESTED TERMS IN CARNIVOROUS SHORE BIRDS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
F_{WI}	Fraction of diet comprised of water invertebrates	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of water invertebrates. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applided to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertaintiy and may over-estimate exposure from ingestion of a single dietary item. (3) The defalut value for an equal diet introduces uncertainity and may over- or under- estimate exposure when applied to site-specific receptors.
C_{HPF}	Concentration in herbivorous and planktivorous fish	mg/kg	**Varies (calculated - Table F-1-13)** This variable is site-specific and COPC-specific; it is calculated using the equation in F-1-16. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. (2) The data set used to calculate BCF_{fish} is based on a limited number of test organisms and therefore may over- or under-estimate exposure when applied to site-specific organisms.
P_{HPF}	Proportion of herbivorous and planktivorous fish diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.

TABLE F-2-13

COPC DOSE INGESTED TERMS IN CARNIVOROUS SHORE BIRDS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
F_{HPF}	Fraction of diet comprised of herbivorous and planktivorous fish	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of herbivorous/piscivorous fish. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applided to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertaintiy and may over-estimate exposure from ingestion of a single dietary item. (3) The defalut value for an equal diet introduces uncertainity and may over- or under- estimate exposure when applied to site-specific receptors.
C_{OB}	Concentration of COPC in omnivorous birds	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-6)** This variable is site-specific and COPC-specific; it is calculated using the equation in Table F-1-6. Uncertainties associated with this variable include: (1) Variables C_{sed} and C_{wctot} are COPC- and site-specific. (2) Variables $BCF_{S\text{-}OB}$ and $BCF_{W\text{-}OB}$ are based on biotransfer factors for chicken ($Ba_{chicken}$), and receptor specific ingestion rates, and therefore may introduce uncertainty when used to compute concentrations for site-specific omnivorous birds.

TABLE F-2-13

COPC DOSE INGESTED TERMS IN CARNIVOROUS SHORE BIRDS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
P_{OB}	Proportion of omnivorous bird in diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{OB}	Fraction of diet comprised of omnivorous birds	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of omnivorous birds. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.
C_{OF}	Concentration of COPC in omnivorous fish	mg COPC/kg FW tissue	**Varies (calculated - Table F-1-16)** This variable is site-specific and COPC-specific; it is calculated using the equation in F-1-16. Uncertainties associated with this variable include: (1) C_{dw} values are COPC- and site-specific. (2) The data set used to calculate BCF_{fish} is based on a limited number of test organisms and therefore may over- or under-estimate exposure when applied to site-specific organisms.

TABLE F-2-13

COPC DOSE INGESTED TERMS IN CARNIVOROUS SHORE BIRDS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
P_{OF}	Proportion of omnivorous fish diet that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of the dietary food item that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for all food types when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated food ingested by a species depends on food availability, diet composition, and animal behavior. Therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and may overestimate the proportion of contaminated food ingested.
F_{OF}	Fraction of diet comprised of omnivorous fish	unitless	**0 to 1** This variable is species- and site-specific, and depends on the percentage of the diet that is comprised of omnivorous fish. The default value for a screening level ecological risk assessment is 100 percent for computing concentration based on an exclusive diet. For calculating an equal diet, F_{diet} is determined based on the number of dietary components in the total diet. The application of an equal diet is further discussed in Chapter 5. Uncertainties associated with this variable include: (1) The actual proportion of the diet that is comprised of a specific dietary item depends on several factors including: food availability, animal behavior, species composition, and seasonal influences. These uncertainties may over- or under- estimate F_{diet} when applied to site-specific receptors. (2) The default value of 100 percent for an exclusive diet introduces uncertainty and may over-estimate exposure from ingestion of a single dietary item. (3) The default value for an equal diet introduces uncertainty and may over- or under- estimate exposure when applied to site-specific receptors.

TABLE F-2-13

COPC DOSE INGESTED TERMS IN CARNIVOROUS SHORE BIRDS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{sed}	COPC concentration in bed sediment	mg COPC/kg DW sediment	**Varies (calculated - Table B-2-19)** This equation calculates the concentration of COPCs in bed sediments. Uncertainties associated with this equation include the following: (1) The default variable values recommended for use in the equation in Table B-2-19 may not accurately represent site-specific water body conditions. The degree of uncertainty associated with default variable values is expected to be limited either because the probable ranges for these variables are narrow or because information allowing reasonable estimates is generally available. (2) Uncertainties associated with variables f_{bs}, C_{wctot} and Kd_{bs} are largely associated with the use of default *OC* content values in their calculation. The uncertainty may be significant in specific instances, because *OC* content is known to vary widely in different locations in the same medium. This variable is site-specific.
$IR_{S\text{-}CSB}$	Sediment ingestion rate for carnivorous shorebird	kg DW/kg BW-day	**Varies** This variable is site-, receptor-, and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. Uncertainties associated with this variable include the following: (1) IR_S values may under- or over-estimate BCF_S when applied to site-specific organisms.
P_S	Portion of ingested bed sediment that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of soil ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used for a screening level risk assessment when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated soil ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of soil ingested that is contaminated will likely be overestimated.

TABLE F-2-13

COPC DOSE INGESTED TERMS IN CARNIVOROUS SHORE BIRDS IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

Variable	Description	Units	Value
C_{wctot}	Total COPC concentration in water column	mg COPC/L water (or g COPC/m^3 water)	**Varies (calculated - Table B-2-17)** This variable is COPC- and site-specific and is calculated using Table B-2-17. Uncertainties associated with this equation include the following: (1) All of the variables in the equation in Table B-2-17 are COPC- and site-specific. Therefore, the use of default values rather than site-specific values, for any or all of these variables, will contribute to the under- or overestimation of C_{wctot}. (2) Uncertainty associated with f_{wc} is largely the result of uncertainty associated with default OC content values. Uncertainties may also be associated with the variable L_T and k_{wt}. The degree of uncertainly associated with the variables d_{wc} and d_{bs} is expected to be minimal either because information for estimating a variable (d_{wc}) is generally available or because the probable range for a variable (d_{bs}) is narrow. The uncertainty associated with the variables f_{wc} and C_{wctot} is associated with estimates of *OC* content. Because *OC* content values can vary widely for different locations in the same medium, the uncertainty associated with using default *OC* values may be significant in specific cases.
$IR_{W\text{-}CSB}$	Water ingestion rate for carnivorous shorebird	L/kg BW-day	**Varies** This variable is receptor- and habitat-specific, and is discussed in Chapter 5. Ingestion rates for example measurement receptors are presented in Chapter 5, Table 5-1. The following uncertainty is associated with this variable: (1) Water ingestion rates are strongly influenced by animal behavior and environmental factors and may over- or under- estimate $BCF_{W\text{-}CSB}$ to an unknown degree.
P_W	Portion of ingested water that is contaminated	unitless	**0 to 1** **Default: 1** This variable is species- and site-specific, and depends on the percentage of water ingested that is contaminated. U.S. EPA OSW recommends that a default value of 1.0 be used when site specific information is not available. The following uncertainty is associated with this variable: (1) The actual amount of contaminated water ingested by species depends on site-specific information, receptor homerange, and animal behavior; therefore, the default value of 100 percent may not accurately reflect site-specific conditions, and the proportion of ingested water that is contaminated will likely be overestimated.

TABLE F-2-13

COPC DOSE INGESTED TERMS IN CARNIVOROUS SHORE BIRDS
IN BRACKISH/INTERMEDIATE MARSH, SALTMARSH, AND FRESHWATER/WETLAND FOOD WEBS

REFERENCES AND DISCUSSIONS

U.S. EPA. 1993. *Wildlife Exposure Factor Handbook.* Volumes I and II. Office of Research and Development. EPA/600/R-93/187a

APPENDIX G

STATE NATURAL HERITAGE PROGRAMS

Screening Level Ecological Risk Assessment Protocol

August 1999

APPENDIX G

TABLE OF CONTENTS

APPENDIX G

STATE NATURAL HERITAGE PROGRAMS

(Page 1 of 3)

Alabama Natural Heritage Program Huntingdon College 1500 East Fairview Avenue Montgomery, AL 36106 334-834-4519 334-834-5439 (Fax) Department of Conservation & Natural Resources Game and Fish Divison Folsom Administration Building 64 N. Union Street, Room 421 Montgomery, AL 36130 334-242-3484 334-242-0098 (Fax)	Alaska Natural Heritage Program University of Alaska Anchorage 707 A Street Anchorage, AK 99501 907-257-2702 907-258-9139 (Fax)	Arizona Heritage Data Management System Arizona Game & Fish Department WM-H 2221 W. Greenway Road Phoenix, AZ 85023 602-789-3612 602-789-3928 (Fax)	Arkansas Natural Heritage Commission Suite 1500, Tower Building 323 Center Street Little Rock, AR 72201 501-324-9150 501-324-9618 (Fax)
California Natural Heritage Division Department of Fish & Game 1220 S Street Sacramento, CA 95814 916-322-2493 916-324-0475 (Fax)	Colorado State University 254 General Services Building Fort Collins, CO 80523 970-491-1309 970-491-3349 (Fax)	Connecticut Natural Diversity Database Natural Resources Center Department of Environmental Protection 79 Elm Street, Store Level Hartford, CT 06106-5127 860-424-3540 860-424-4058 (Fax)	Delaware Natural Heritage Program Division of Fish & Wildlife Department of Natural Resources & Environmental Control 4876 Hay Point Landing Road Smyrna, DA 19977 302-653-2880 302-653-3431 (Fax)
District of Columbia Natural Heritage Program 13025 Riley's Lock Road Poolesville, MD 20837 301-427-1354 301-427-1355 (Fax)	Florida Natural Areas Inventory 1018 Thomasville Road Suite 200-C Tallahassee, FL 32303 904-224-8207 904-681-9364 (Fax)	Georgia Natural Heritage Program Wildlife Resources Division Georgia Department of Natural Resources 2117 U.S. Highway 278 S.E. Social Circle, GA 30279 706-557-3032 or 770-918-6411 706-557-3033 or 706-557-3040 (Fax)	Hawaii Natural Heritage Program The Nature Conservancy of Hawaii 1116 Smith Street, Suite 201 Honolulu, HI 96817 808-537-4508 808-545-2019 (Fax)
Idaho Conservation Data Center Department of Fish & Game 600 South Walnut Street, Box 25 Boise, ID 83707-0025 208-334-3402 208-334-2114 (Fax)	Illinois Natural Heritage Division Department of Natural Resources Division of Natural Heritage 524 South Second Street Springfield, IL 62701-1787 217-785-8774 217-785-8277 (Fax)	Indiana Natural Heritage Data Center Division of Nature Preserves Department of Natural Resources 402 West Washington Street, Room W267 Indianapolis, IN 46204 317-232-4052 317-233-0133 (Fax)	Iowa Natural Areas Inventory Bureau of Preserves & Ecological Services Department of Natural Resources Wallace State Office Building Des Moines, IA 50319-0034 515-281-8524 (Fax)

APPENDIX G

STATE NATURAL HERITAGE PROGRAMS

(Page 2 of 3)

Kansas Natural Heritage Inventory Kansas Biological Survey 2041 Constant Avenue Lawrence, KS 66047-2906 913-864-3453 913-864-5093 (Fax)	Kentucky Natural Heritage Program Kentucky State Nature Preserves Commission 801 Schenkel Lane Frankfort, KY 40601 502-573-2886 502-573-2355 (Fax)	Louisiana Natural Heritage Program Department of Wildlife & Fisheries P.O. Box 98000 Baton Rouge, LA 70898-9000 504-765-2821 504-765-2607 (Fax)	Maine Natural Areas Program Department of Conservation (FedEx/UPS: 159 Hospital Street) 93 State House Station Augusta, ME 04333-0093 207-287-8044 207-287-8040 (Fax)
Maryland Heritage & Biodiversity Conservation Programs Department of Natural Resources Tawes State Office Building, E-1 Annapolis, MD 21401 410-974-2870 410-974-5590 (Fax)	Massachusetts Natural Heritage & Endangered Species Program Division of Fisheries & Wildlife Route 135 Westborough, MA 01581 508-792-7270 508-792-7275 (Fax)	Michigan Natural Features Inventory Mason Building, 5th Floor Box 30444 (FedEx/UPS: 530 W. Allegan, 48933) Lansing, MI 48909-7944 517-373-1552 517-373-6705 (Fax)	Minnesota Natural Heritage & Nongame Research Department of Natural Resources 500 Lafayette Road, Box 7 St. Paul, MN 51555 612-297-4964 612-297-4961 (Fax)
Mississippi Natural Heritage Program Museum of Natural Science 111 North Jefferson Street Jackson, MS 39201 601-354-7303 601-354-7227 (Fax)	Missouri Natural Heritage Division Missouri Department of Conservation P.O. Box 180 (FedEx: 2901 West Truman Blvd.) Jefferson City, MO 65102-0180 573-751-4115 573-526-5582 (Fax)	Montana Natural Heritage Program State Library Building 1515 E. 6th Avenue Helena, MT 59620 406-444-3009 406-444-0581 (Fax)	Nebraska Natural Heritage Program Game and Parks Commission 2200 North 33rd Street P.O. Box 30370 Lincoln, NE 68503 402-471-5421 402-471-5528 (Fax)
Nevada Natural Heritage Program Department of Conservation & Natural Resources 1550 E. College Parkway, Suite 145 Carson City, NV 89710 702-687-4245 702-885-0868 (Fax)	New Hampshire Natural Heritage Inventory Department of Resources & Economic Development 172 Pembroke Street P.O. Box 1856 Concord, NH 03302 603-271-3623 603-271-2629 (Fax)	New Jersey Natural Heritage Program Office of Natural Lands Management 22 South Clinton Ave., CN404 Trenton, NJ 08625-0404 609-984-1339 609-984-1427 (Fax)	New Mexico Natural Heritage Program University of New Mexico 2500 Yale Boulevard, SE, Suite 100 Albuquerque, NM 87131-1091 505-277-1991 505-277-7587 (Fax)
New York Natural Heritage Program Department of Environmental Conservation 700 Troy-Schenectady Road Latham, NY 12110-2400 518-783-3932 518-783-3916 (Fax)	North Carolina Heritage Program NC Department of Environment, Health & Natural Resources Division of Parks & Recreation P.O. Box 27687 Raleigh, NC 27611-7687 919-733-7701 919-715-3085 (Fax)	North Dakota Natural Heritage Inventory North Dakota Parks and Recreation Department 1835 Bismarck Expressway Bismarck, ND 58504 701-328-5357 701-328-5363 (Fax)	Ohio Natural Heritage Data Base Division of Natural Areas & Preserves Department of Natural Resources 1889 Fountain Square, Building F-1 Columbus, OH 43224 614-265-6453 614-267-3096 (Fax)

APPENDIX G

STATE NATURAL HERITAGE PROGRAMS

(Page 3 of 3)

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APPENDIX H

TOXICOLOGICAL PROFILES

Screening Level Ecological Risk Assessment Protocol

August 1999

APPENDIX H

TOXICOLOGICAL PROFILES

Profile **Page**

APPENDIX H

TOXICOLOGICAL PROFILES

ACETONE

1.0 SUMMARY

Acetone is a highly volatile organic compound. Volatilization and biodegradation are the major fate processes affecting acetone released to soil, surface water, and sediment. Routes of exposure for wildlife include ingestion, inhalation, and dermal uptake. Acetone is not bioconcentrated by aquatic organisms, and is not bioaccumulated by mammals and birds. Therefore, it does not bioaccumulate in aquatic or terrestrial food chains.

The following is a profile of the fate of acetone in soil, surface water and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER AND SEDIMENT

Volatilization and leaching are the two primary transport properties affecting the fate of acetone in soils (HSDB 1997). Volatilization is more significant than leaching. The extent of leaching depends on soil characteristics. Evidence also suggests that acetone rapidly degrades in soil (HSDB 1997).

Volatilization and biodegradation are the major fate processes affecting the fate of acetone in surface water. The volatilization half-life for acetone from a model river is approximately 18 hours when estimated using 1-meter depth, a current of 1 m/second, and wind velocity of 3 m/second (Thomas 1982). In addition, acetone does not partition well to sediments because it is highly soluble in water. Dispersion of acetone from the water column to sediment and suspended solids in water is likely to be insignificant, due to the complete miscibility of acetone in water.

Biodegredation is the most significant degradation process of acetone in water (Rathbun et al. 1982). Studies on wastewater have shown that aquatic microbial communities quickly acclimate to acetone, and rapidly biodegrade it (Urano and Kato 1986a,b). When tested in seawater, acetone was biodegraded much slower than when tested in freshwater (Takemoto et al. 1981).

Photolysis as a degradation process for acetone in water is insignificant. Studies have shown that photodecomposition was not observed when acetone contaminated distilled or natural water was exposed to sunlight for 2-3 days (Rathbun et al. 1982).

3.0 FATE IN ECOLOGICAL RECEPTORS

For most aquatic systems, acetone will exist in water rather than sediment, due to acetone's high water solubility and low sediment adsorption coefficient. Bioaccumulation does not occur in aquatic organisms as suggested by the low log K_{ow} value for acetone (Rathbun et al. 1982). Adult haddock tested under static conditions at 7.9°C showed a bioconcentration factor of 1 for acetone (Rustung et al. 1931). Biomagnification along the aquatic food chain is also considered insignificant for acetone as suggested by the low K_{ow} value.

Acetone is a highly volatile compound and may be inhaled in large quantities. Acetone is very water soluble, so it is quickly absorbed following inhalation into the blood stream and dispersed throughout the body. A large portion of acetone is excreted primarily unchanged through the lungs and urine, with only a small portion reduced and excreted as carbon dioxide (Encyclopedia of Occupational Health and Safety 1983). Because acetone is quickly eliminated, wildlife receptors will not accumulate it in tissues.

No information was available on the fate of acetone after exposure by birds or plants.

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ACRYLONITRILE

1.0 SUMMARY

Acrylonitrile is a highly water soluble volatile organic compound. Volatilization and biodegradation are the major fate processes affecting acrylonitrile released to surface soil, surface water, and sediment. Routes of exposure for wildlife include ingestion, inhalation, and dermal uptake. Acrylonitrile is not bioconcentrated by aquatic organisms, and is not bioaccumulated by mammals and birds. Therefore, it does not bioaccumulate in aquatic or terrestrial food chains.

The following is a profile of the fate of acrylonitrile in soil, surface water, and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in surface soil, surface water, and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

Due to its high water solubility, acrylonitrile is highly mobile in moist soils (EPA 1987). Adsorption into the soil is considered insignificant (Kenaga 1980). Evaporation of acrylonitrile from dry soils is expected to occur rapidly because of its high vapor pressure (Norris 1967; EPA 1987) and high Henry's Law constant (Meylan 1991).

Acrylonitrile is readily soluble in water and does not strongly adsorb to soil or sediment (Klein et al. 1957; ATSDR 1990). Acrylonitrile biodegrades rapidly in water (Miller and Villaume 1978; EPA 1987). Aerobic microorganisms readily degrade acrylonitrile, particularly if acclimation time is allowed (Cherry et al. 1956; Stover and Kincannon 1983; Mills and Stack 1954, 1955).

Acrylonitrile rapidly volatilizes from surface water. A volatilization half-life of 1-6 days in water has been estimated (Thomas 1982; HSDB 1997).

3.0 FATE IN ECOLOGICAL RECEPTORS

Based on experimental and estimated bioconcentration factors, the bioconcentration of acrylonitrile in aquatic organisms is not believed to be significant (Kenaga 1980). A steady-state bioconcentration factor

(BCF) of 48 was measured in bluegill sunfish (Barrows et al. 1978). The estimated average BCF for edible portions of freshwater and marine species was approximately 30 based on the relative proportion of fat in sunfish and other organisms (EPA 1980). Also, based on a low log K_{ow}, acrylonitrile is estimated to show low bioconcentration in aquatic organisms (Verschueren 1983; Kenaga 1980).

Acrylonitrile is readily absorbed into the body through lung and intestinal mucosa following inhalation, ingestion, or dermal contact (Clayton and Clayton 1982). Once absorbed into the body, acrylonitrile is distributed throughout the body to the major organs (Pilon et al. 1988a). Following a single oral dose of radiolabeled acrylonitrile, rapid distribution of acrylonitrile and its metabolites was shown in all tissues of rats (Ahmed et al. 1982, 1983; Silver et al. 1987; Young et al. 1968). Another metabolic pathway includes the formation of CO_2 which is excreted via the lungs (Young et al. 1968). The rate of acrylonitrile metabolism is inconclusive; however, evidence suggests that it is rapid (Pilon et al. 1988b; Ghanayem and Ahmed 1982; Miller and Villaume 1978). Values representing the amount of acrylonitrile metabolized range from 4% to 30% (IARC 1979).

No information was available on the fate of acrylonitrile after exposure by birds or plants.

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ALUMINUM

1.0 SUMMARY

In nature, aluminum does not exist in the elemental state, but partitions between the liquid and solid phases by forming complexes with various compounds. Aluminum adsorbs to clays and suspended solids in water. Exposure routes for aquatic organisms include ingestion, gill uptake and dermal contact. Aluminum bioconcentrates in aquatic organisms. Exposure routes for mammals include ingestion, inhalation and dermal exposure; however, regardless of the route of exposure, aluminum is poorly absorbed by mammals. Aluminum is not readily metabolized. Aluminum causes pulmonary and developmental effects. Aluminum uptake by plants varies between species, resulting in differing rates of bioconcentration in plant tissues.

The following is a profile of the fate of aluminum in soil, surface water and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, surface water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER AND SEDIMENT

Aluminum does not exist as a free metal in nature due to its reactivity, but rather partitions between the solid and liquid phases by reacting with water, chloride, fluoride, sulfate, nitrate, phosphate, humic materials and clay (Bodek et al. 1988). Soils with a greater mineral content result in reduced mobility of aluminum (James and Riha 1989).

In water, aluminum forms relatively water-insoluble complexes, or is found as a water-soluble complex. Aluminum adsorbs to suspended solids and sediment. If large amounts of organic matter or fulvic acid are present, aluminum binds to them (Brusewitz 1984). In water, aluminum undergoes hydrolysis to form hydroxy aluminum species (Snoeyink and Jenkins 1980). The pH of the water determines which hydrolysis products are formed.

3.0 ECOLOGICAL RECEPTORS

Exposure routes for aquatic organisms include ingestion, gill uptake, and dermal absorption. Aluminum bioconcentrates in aquatic species (Cleveland et al. 1989).

Exposure routes for mammals include ingestion, inhalation and dermal exposure. Aluminum is poorly absorbed. Aluminum is distributed to the brain (Santos et al. 1987), bone, muscle and kidneys (Greger and Donnaubauer 1986). No studies were located that described excretion of aluminum in animals; however in humans, absorbed aluminum is excreted primarily through the kidney (Gorsky et al. 1979).

Information was not available on the fate of aluminum in birds.

Aluminum is taken up by plants (Brusewitz 1984). Some plants bioaccumulate aluminum in the root tissues. Plant uptake of aluminum and the transport to stems and leaves varies considerably between species (Kabata-Pendias and Pendias 1984).

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ANTIMONY

1.0 SUMMARY

Antimony binds to soil and particulates and is oxidized by bacteria in soil. Exposure routes for aquatic organisms include ingestion and gill uptake. Antimony bioconcentrates in aquatic organisms. Exposure routes for mammals include ingestion and inhalation. It does not biomagnify in terrestrial food chains. Antimony is not significantly metabolized and is excreted in the urine and the feces. Antimony causes reproductive, pulmonary and hepatic effects in mammals. Antimony uptake by plants occurs following surface deposition.

The following is a profile of the fate of antimony in soil, surface water and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, surface water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER AND SEDIMENT

Antimony binds to soil, particularly to particles containing iron, manganese, or aluminum Ainsworth 1988). In water, antimony is oxidized when exposed to atmospheric oxygen (Parris and Brinckman 1976).

3.0 ECOLOGICAL RECEPTORS

Exposure routes for aquatic organisms include ingestion and gill uptake. Antimony bioconcentrates in aquatic organisms (ACQUIRE 1989; Callahan et al. 1979; EPA 1980).

Exposure routes for mammals include ingestion and inhalation (Groth et al. 1986, EPA 1988). Dermal absorption is low (Myers et al. 1978) and absorption from the respiratory tract is dependent on particle size (Thomas et al. 1973). Following absorption, antimony is distributed to the liver, kidney, bone, lung, spleen and thyroid (Sunagawa 1981; Ainsworth 1988). Antimony is excreted in the urine and the feces (Felicetti et al. 1974). Antimony does not biomagnify in the food chain (Ainsworth 1988). Data regarding the amount of antimony that reaches the site of action and assimilation efficiency were not available.

Information was not available on the fate of antimony in birds.

Antimony is taken up by plants following surface deposition, with uptake from soil dependent on the solubility of the antimony in the soil (Ainsworth 1988).

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ARSENIC

1.0 SUMMARY

Arsenic, because of its complex chemistry, exists in the environment in many different inorganic and organic forms, which have different toxicological and physicochemical properties. Inorganic arsenic exists as either the trivalent (3+) form or the pentavalent (5+) form. The inorganic trivalent arsenic forms are more toxic than the pentavalent forms. Elemental arsenic (the metalloid -0+) is essentially nontoxic even at high intakes.

Arsenic in soil is usually tightly bound. The bioconcentration potential in soil invertebrates and aquatic species is low. Biomagnification through the food chain is minimal because once ingested, arsenic is metabolized to methylated compounds that are rapidly excreted. Absorbed arsenic is distributed to all tissues where it interferes with normal enzymatic activity or disrupts the functioning of other cellular macromolecules. Evaluation of the potential for toxicity from exposure to low levels of arsenic is complicated by the current understanding that arsenic is an essential element in some mammalian species, and that arsenic deficiency may result in adverse reproductive and developmental effects.

The following is a profile of the fate of arsenic in soil, surface water and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, surface water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

The dominant form of arsenic in soil and its transport are largely dependent on the physical characteristics of the soil matrix. Insoluble arsenic compounds, such as arsenic trioxide, bind tightly to organic matter in soil or sediment (EPA 1984; ATSDR 1993). Various forms of arsenic in soil are interconverted by chemical reactions and microbial activity. Soil microorganisms convert small amounts of arsenic to volatile arsines. These volatile arsines are released to the air, become adsorbed to particles, and are redeposited (ATSDR 1993) or, under certain conditions, react to form oxides (Ghassemi et al. 1981).

The bioavailability of arsenic in soil is inversely proportional to the organic carbon and clay content of the soil matrix. Arsenic in soil is directly taken up by plants and soil microbes and invertebrates, and indirectly taken up by terrestrial receptors via ingestion.

In surface water, soluble inorganic arsenate (As5+) predominates under normal conditions and is more stable than arsenite (EPA 1980a). Movement and partitioning of arsenic in water depends on the chemical form of arsenic and on interactions with other materials present (Callahan et al. 1979). Soluble forms of arsenic remain dissolved in the water column or adsorb onto sediments or soils, especially those containing clays, iron oxides, aluminum hydroxides, manganese compounds, and organic matter (Callahan et al. 1979; Welch et al. 1988). Sediment bound arsenic is released back into the water by chemical or biological interconversions. This interconversion is influenced by the Eh (the oxidation-reduction potential), pH, temperature, other metals, salinity, and biota (Callahan et al. 1979). Arsenate is transformed by microbes to arsenite and methylated arsenicals (Benson 1989; Braman and Foreback 1973).

3.0 ECOLOGICAL RECEPTORS

Exposure routes for aquatic organisms include gill uptake, ingestion of arsenic suspended on particles in the water column or deposited in sediment, and ingestion of plant matter and lower trophic level aquatic species. Arsenic bioconcentration in aquatic organisms is low (Spehar et al. 1980; EPA 1980b). Fish and shellfish rapidly metabolize arsenic to non-toxic forms (EPA 1984, Garcia-Vargas and Cebrian 1996; ATSDR 1993). Biomagnification does not readily occur in aquatic food chains (Callahan et al. 1979).

Soil invertebrates are directly exposed to arsenic found in soil and soil pore water. Exposure routes for soil invertebrates include ingestion and dermal absorption. Arsenic bioconcentration in soil invertebrates is low (Rhett et al. 1988).

The majority of ecological mammalian exposure occurs through ingestion. The oral absorption efficiency is dependent on the form of arsenic, its solubility, and the media ingested. Soluble arsenic compounds in aqueous solution are more readily absorbed from the gastrointestinal tract than insoluble compounds. Absorption from water ingested is approximately 85%. Inorganic arsenic in food sources is expected to be readily bioavailable with absorption rates of greater than 85% expected. Once absorbed, arsenic is readily transported throughout the body with little tendency to accumulate preferentially in any one internal organ

(ATSDR 1993). Dermal absorption is a minor route of exposure with absorption estimated at 0.1% (ATSDR 1993).

Metabolism of arsenic occurs primarily in the liver. The methylated metabolites are less toxic than the inorganic precursors, and metabolism results in lower tissue retention of inorganic arsenic (Marafante and Vahter 1984, 1986, 1987; Marafante et al. 1985). Inorganic arsenic and its methylated products are rapidly eliminated.

The toxicokinetic data for arsenic indicate there is little potential for bioaccumulation in animal tissue exposed to doses that are below the level required to saturate detoxifying methylation reactions. The level of biomagnification in mammals depends on the diet of the animal. Herbivores have a low arsenic biomagnification rate due to the general lack of transport of arsenic from soil to above ground plant parts. Omnivores have a higher biomagnification rate based on the higher proportion of soil invertebrates in their diet. Carnivores have the highest biomagnification rate due to their diet of aquatic invertebrates, small mammals, and fish and the incidental ingestion of soil. However, arsenic is rapidly metabolized in mammalian species, therefore, arsenic does not readily bioaccumulate in mammals.

Exposure routes for avian receptors include ingestion of surface water, soil, soil and aquatic invertebrates, and plant material. Absorption studies specific to avian species are not available. Based on mammalian absorption (ATSDR 1993), avian absorption can be assumed to be 85% absorption from water, 30% to 40% absorption from soil, and 85% absorption from food sources.

Arsenic uptake by plants depends on the form of arsenic and the type of soil. The higher the soil's organic carbon and clay content the more the arsenic will bind to the soil and, therefore, less arsenic is available for uptake by plant roots. That which is readily taken up by the plant is accumulated in the roots. Arsenite (3+) is highly toxic to cell membranes and, therefore, not readily translocated once taken up; arsenate (5+) is less toxic and, therefore, more readily translocated after uptake (ORNL 1996; Speer 1973). Rice, most legumes, and members of the bean family are sensitive to arsenic in most forms, with spinach being the most sensitive plant (Woolson et al 1975).

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BERYLLIUM

1.0 SUMMARY

In environmental media, beryllium usually exists as beryllium oxide. Beryllium has limited solubility and mobility in sediment and soil. Exposure routes for aquatic organisms include ingestion and gill uptake. Beryllium does not bioconcentrate in aquatic organisms. Beryllium is toxic to warm water fish, especially in soft water. Exposure routes for mammalian species include inhalation. Mammals exposed via inhalation exhibit pulmonary effects which may last long after exposure ceases.

The following is a profile of the fate of beryllium in soil, surface water and sediment, and the fate after uptake by biological receptors. Section 2 discusses the environmental fate and transport in soil, surface water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

Beryllium adsorbs to clays at low pH, precipitates as insoluble complexes at higher pH, and has limited solubility in soil (Callahan et al. 1979). Chemical reactions in soil transform one beryllium compound into another (ATSDR 1993). Reactions in soil include hydrolysis of soluble salts, anion exchange, and complexation with ligands such as humic substances (ATSDR 1993).

In water, beryllium is speciated often by hydrolysis in which soluble beryllium salts are hydrolyzed to form relatively insoluble beryllium hydroxide (Callahan et al. 1979). Beryllium is not volatilized from water (ATSDR 1993). Beryllium is retained in an insoluble and immobile form in sediment (EPA 1980).

3.0 ECOLOGICAL RECEPTORS

Beryllium uptake from water is low, resulting in low bioconcentration rates (EPA 1980; Callahan et al. 1979). Biomagnification of beryllium in aquatic food chains does not occur (Fishbein 1981).

In mammals, beryllium compounds are absorbed primarily through the lung (ATSDR 1993). Beryllium is poorly absorbed from the gastrointestinal tract, and is not absorbed through intact skin to any significant degree

(ATSDR 1993). Beryllium is distributed to the liver, skeleton, tracheobronchial lymph nodes, and blood (Finch et al. 1990). Beryllium is not biotransformed, but soluble beryllium salts are partially converted to less soluble forms in the lung (Reeves and Vorwald 1967). Excretion is predominantly via the feces (Finch et al. 1990). Data regarding the amount of beryllium that reaches the site of action or assimilation efficiency were not located.

Information was not available on the fate of beryllium in birds.

Beryllium uptake by plants occurs when beryllium is present in the soluble form. The highest levels of beryllium are found in the roots, with lower levels in the stems and foliage (EPA 1985).

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BIS(2-ETHYLHEXYL)PHTHALATE

1.0 SUMMARY

Bis(2-ethylhexyl)phthalate (BEHP) is a high molecular weight, semi-volatile organic compound. BEHP adsorbs strongly to soil and sediment, and it may be biodegraded in aerobic environments. It has a low water solubility and low vapor pressure. It does not undergo significant photolysis, hydrolysis, or volatilization in soil or water. Receptors may be exposed to BEHP by the oral, inhalation, and dermal routes. BEHP bioconcentration in aquatic organisms is generally low, therefore significant food chain biomagnification in upper-trophic-level fish is unlikely. Mammalian and avian wildlife can metabolize and eliminate BEHP, therefore, it does not biomagnify in these receptors.

The following summarizes the fate of BEHP in surface soil, surface water and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate after released to surface soil, surface water, and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER AND SEDIMENT

BEHP adsorbs strongly to soil and does not undergo significant volatilization or photolysis (HSDB 1997). Limited information indicates that, under aerobic conditions, degradation in soil may occur (Hutchins et al. 1983; Mathur 1974). However, because BEHP adsorbs strongly to soil, biodegradation is slow (Wams 1987). Biodegradation in anaerobic conditions is slower than under aerobic conditions (Johnson et al. 1984).

BEHP has a low water solubility. In surface water environments, adsorption is the major mechanism affecting the concentration of BEHP. BEHP strongly adsorbs to suspended solids and sediments (Al-Omran and Preston 1987; Sullivan et al. 1982; Wolfe et al. 1980). However, in marine environments, adsorption to sediments may be decreased because BEHP is not as soluble in salt water when compared to fresh water (Al-Omran and Preston 1987). BEHP may also form complexes with fulvic acid, potentially increasing its mobility in aquatic environments (Johnson et al. 1977).

In aquatic environments, biodegradation is the primary route of degradation. BEHP is biodegraded in aerobic conditions; however, under anaerobic conditions, biodegradation is limited (O'Connor et al. 1989; Tabek et al. 1981; O'Grady et al. 1985). A half-life of approximately one month, due to microbial biodegradation has been reported for BEHP in river water (Wams 1987). BEHP does not undergo significant hydrolysis or photolysis in aquatic environments (Callahan et al. 1979). A hydrolysis half-life of 2,000 years has been estimated (Callahan et al. 1979); and in water a photolysis half-life of 143 days has been reported (Wolfe et al. 1980). BEHP does not significantly volatilize from water, with an half-life of 15 years reported (Callahan et al. 1979).

3.0 FATE IN ECOLOGICAL RECEPTORS

Aquatic receptors may be exposed through ingestion of contaminated food or water, dermal exposure, or in the case of fish, by direct contact of the gills with the surrounding water. Based on its low water solubility and high soil partition coefficient (ATSDR 1993), dietary uptake is the most significant route of exposure anticipated for BEHP.

Based on its high log Kow value, BEHP is expected to accumulate in aquatic species (Barrows et al.1980; Mayer 1977). Invertebrates will bioconcentrate BEHP from surface water and from sediment. The level of bioconcentration is receptor-specific, because some invertebrates can metabolize BEHP, while some have limited capability (Sanders et al. 1973). Under continuous exposure conditions, fish will bioconcentrate BEHP to levels moderately higher than the concentration in surface water (Mehrle and Mayer 1976). BEHP has a short half-life in fish, indicating that it is quickly eliminated (Park et al. 1990). Fish eliminate BEHP by metabolizing it to polar byproducts, which are quickly excreted (Melancon and Lech 1977; Menzie 1980). Therefore, food chain accumulation and biomagnification of BEHP in aquatic food webs is not significant (Callahan et al. 1979; Johnson et al. 1977; Wofford et al. 1981).

BEHP is absorbed by mammals following oral (Astill 1989; Rhodes et al. 1986) or dermal exposure (Melnick et al. 1987), with oral exposure being the route with the greatest absorption efficiency in laboratory animals. In laboratory animals, small amounts of BEHP have been shown to be absorbed following dermal exposure (Melnick et al. 1987). Following oral exposure, it has been reported that a portion of the BEHP is hydrolyzed in the small intestine to 2-ethylhexanol and mono(ethylhexyl)phthalate

which is subsequently absorbed (Albro, et al. 1982). Following absorption, BEHP is distributed primarily to the liver and kidney, and in some species, to the testes (Rhodes et al. 1986).

In mammals, BEHP is metabolized by tissue esterases that hydrolyze one of the ester bonds resulting in the formation of mono(2-ethylhexyl)phthalate and 2-ethylhexanol. Small amounts of mono(2-ethylhexyl)phthalate may be further hydrolyzed to form phthalic acid; however, the majority undergoes aliphatic side chain oxidation followed by alpha- or beta-oxidation. These oxidized products may then be conjugated with glucuronic acid and excreted (Albro 1986). Metabolites of BEHP are excreted in both the urine and the feces (Astill 1989; Short et al. 1987; Ikeda et al. 1980).

BEHP may evaporate from the leaves of plants. In one study, using a closed terrestrial simulation chamber, BEHP was applied to the leaves of *Sinapis alba*. Evaporation rates from the leaves were <0.8 ng/cm^2-hr for a time interval of 0–1 days and <0.5 ng/cm^2-hr for a time interval of 8–15 days (Loekke and Bro-Rasumussen 1981). Uptake of BEHP by plants has also been reported (Overcash et al. 1986).

No data were available on the fate of BEHP in birds.

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CADMIUM

1.0 SUMMARY

Cadmium exists in the elemental (0+) state or the 2+ valance state in nature. Exposure routes for aquatic organisms include ingestion and gill uptake. Freshwater biota are the most sensitive organisms to cadmium exposure, with toxicity inversely proportional to water hardness. Cadmium bioaccumulates in both aquatic and terrestrial animals, with higher bioconcentration in aquatic organisms. Exposure routes for ecological mammalian species include ingestion and inhalation. Cadmium interferes with the absorption and distribution of other metals and causes renal toxicity in vertebrates.

The following is a profile of the fate of cadmium in soil, surface water and sediment, and the fate after uptake by biological receptors. Section 2 discusses the environmental fate and transport in soil, surface water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER AND SEDIMENT

Cadmium has a low vapor pressure and is released from soil to air by entrainment with soil particles (EPA 1980; OHM/TADS 1997). Cadmium compounds in soil are stable and are not subject to degradation (ATSDR 1993). Cadmium compounds can be transformed by precipitation, dissolution, complexation, and ion exchange (McComish and Ong 1988).

Cadmium compounds in aquatic environments are not affected by photolysis, volatilization, or biological methylation (Callahan et al. 1979). Precipitation and sorption to mineral surfaces and organic materials are important removal processes for cadmium compounds (ATSDR 1993). Concentrations of cadmium are generally higher in sediments than in overlying water (Callahan et al. 1979).

3.0 ECOLOGICAL RECEPTORS

Cadmium bioconcentrates in aquatic organisms, primarily in the liver and kidney (EPA 1985). Cadmium accumulated from water is slowly excreted, while cadmium accumulated from food is eliminated more

rapidly (EPA 1985). Metal-binding, proteinaceous, metallothionens appear to protect vertebrates from deleterious effects of high metal body burdens (Eisler 1985).

Exposure routes in ecological mammalian species include ingestion and inhalation, while dermal absorption is negligible (Goodman and Gilman 1985). Absorption and retention of cadmium decreases with prolonged exposure. Cadmium absorption through ingestion is inversely proportional to intake of other metals, especially iron and calcium (Friberg 1979). Cadmium accumulates primarily in the liver and kidneys (IARC 1973). Cadmium crosses the placental barrier (Venugopal 1978). Cadmium does not undergo direct metabolic conversion, but the ionic (+2 valence) form binds to proteins and other molecules (Nordberg et al. 1985). Absorbed cadmium is excreted very slowly, with urinary and fecal excretion being approximately equal (Kjellstrom and Nordberg 1978).

Freshwater aquatic species are most sensitive to the toxic effects of cadmium, followed by marine organisms, birds, and mammals.

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CHROMIUM

1.0 SUMMARY

Chromium exists primarily in the Cr3+ and Cr6+ valence forms in environmental and biological media. It exists in soil primarily in the form of insoluble oxides with very limited mobility. In the aquatic phase, chromium may be in the soluble state or attached to clay-like or organic suspended solids.

Exposure routes for aquatic organisms include ingestion, gill uptake, and dermal absorption. Bioaccumulation occurs in aquatic receptors; biomagnification does not occur in aquatic food chains. Exposure routes for ecological mammalian species include ingestion, inhalation, and dermal absorption. Chromium is not truly metabolized, but undergoes various changes in valence states and binding with ligands and reducing agents in vivo. Elimination of chromium is slow.

The following is a profile of the fate of chromium in soil, surface water and sediment, and the fate after uptake by biological receptors. Section 2 discusses the environmental fate and transport in soil, surface water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

In soil, chromium 3+ is readily hydrolyzed and precipitated as chromium hydroxide. It exists in soil primarily as insoluble oxide with very limited mobility (EPA 1984a, b).

In water, chromium 6+ occurs in the soluble state or as suspended solids adsorbed onto clay-like materials, organics, or iron oxides. Cr6+ persists in water for long periods of time, but is eventually reduced to chromium 3+ by organic matter or other reducing agents in water (Cary 1982).

3.0 ECOLOGICAL RECEPTORS

Exposure routes for aquatic organisms include ingestion, gill uptake, and dermal absorption. Chromium bioconcentrates in aquatic organisms (ATSDR 1993; OHM/TADS 1997; EPA 1985; EPA 1984a). The

biomagnification and toxicity of chromium 3+ is low relative to chromium 6+ because of its low membrane permeability and noncorrosivity. Chromium is not significantly biomagnified in aquatic food chains.

In vertebrates, chromium 3+ is an essential nutrient needed to produce glucose tolerance factor (GTF), which is required for regulation of glucose levels (ATSDR 1993). Exposure routes for ecological mammalian species include ingestion, inhalation, and dermal absorption. Chromium is poorly absorbed from the gastrointestinal tract after oral exposure, but fasting increases the absorption (Chen et al. 1973). Absorbed chromium is distributed to various organs including the liver and spleen (Maruyama 1982 as cited in ATSDR 1993; Witmer et al. 1989, 1991, as cited in ATSDR 1993).

Following inhalation exposure, chromium is distributed to the lung, kidney, spleen, and erythrocytes (Weber 1983; Baetjer et al. 1959). Following dermal exposure, chromium is readily absorbed and is distributed to the blood, spleen, bone marrow, lymph glands, urine, and kidneys. Chromium is not truly metabolized, but undergoes various changes in valence states and binding with ligands and reducing agents in vivo. Elimination of chromium is slow (Langard et al. 1978).

A large degree of accumulation by aquatic and terrestrial plants and animals in the lower trophic levels has been documented, however, the mechanism of this accumulation remains unknown.

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COPPER

1.0 SUMMARY

Copper binds to soils and sediment. Copper is not biodegraded or transformed. Exposure routes for aquatic organisms include ingestion, gill uptake, and dermal absorption. In aquatic organisms, exposures to copper are associated with developmental abnormalities. Copper bioconcentrates in aquatic organisms, however, biomagnification does not occur. Exposure routes for ecological mammalian species include ingestion, inhalation, and dermal absorption. Copper is associated with adverse hematological, hepatic, developmental, immunological, and renal effects in mammals. Copper does not bioaccumulate in mammals.

The following is a profile of the fate of copper in soil, surface water and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, surface water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER AND SEDIMENT

Copper occurs naturally in many animals and plants and is an essential micronutrient. Copper may exist in two oxidation states: +1 or +2. Copper (+1) is unstable and, in aerated water over the pH range of most natural waters (6 to 8), oxidizes to the +2 state. In the aquatic environment, the fate of copper is determined by the formation of complexes, especially with humic substances, and sorption to hydrous metal oxides, clays, and organic materials. The amount of copper able to remain in solution is directly dependent on water chemistry, especially pH and temperature, and the concentration of other chemical species (Callahan et al. 1979; Tyler and McBride 1982; Fuhrer 1986).

The majority of copper released to surface waters settles out or adsorbs to sediments (Harrison and Bishop 1984). Copper is affected by photolysis (Moffett and Zika 1987). Some copper complexes undergo metabolism however, biotransformation of copper is low (Callahan 1979).

3.0 ECOLOGICAL RECEPTORS

Copper bioconcentrates in aquatic organisms. Copper does not biomagnify in aquatic food chains (Heit and Klusek 1985; Perwack et al. 1980).

Copper is absorbed by mammals following ingestion, inhalation, and dermal exposure (Batsura 1969; Van Campen and Mitchell 1965; Crampton et al. 1965). Once absorbed, copper is distributed to the liver (Marceau et al. 1970). Copper is not metabolized. Copper exerts its toxic effects by binding to DNA (Sideris et al. 1988) or by generating free radicals (EPA 1985). Copper does not bioaccumulate in mammals and is excreted primarily in the bile (Bush et al. 1955).

Copper is known to inhibit photosynthesis and plant growth. Because copper is an essential micronutrient for plant nutrition, most adverse effects result from copper deficiency (Adriano 1986).

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CROTONALDEHYDE

1.0 SUMMARY

Crotonaldehyde is a highly volatile, water-soluble, low molecular weight, organic compound. Volatilization is the major fate process for crotonaldehyde in surface water and surface soil. Crotonaldehyde does not bioconcentrate in aquatic organisms and does not accumulate in wildlife. Therefore, food chain transfer is insignificant.

The following summarizes information about the fate of crotonaldehyde in soil, surface water, and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

Crotonaldehyde has a low K_{oc} value, therefore it will not strongly adsorb to soils (Irwin 1988 as cited in ATSDR 1990), and may dissolve in soil water. Crotonaldehyde has a short half-life (Lyman 1982) and it will quickly volatilize from surface soils.

Crotonaldehyde is completely miscible in water and does not dissolve in oils. However, based on its volatilization half-life of about 1 to 2 days (Bowmer et al. 1974; Thomas 1982), crotonaldehyde is expected to quickly volatilize from surface water. The adsorption of crotonaldehyde to suspended solids and sediment is not expected to be significant because of its low K_{oc} value (Lyman 1982).

Aerobic biodegradation may degrade crotonaldehyde at low concentrations in natural water (Bowmer and Higgins 1976; Callahan et al. 1979; Tabak et al. 1981). In addition, data suggest that persistence of crotonaldehyde in aerobic aquatic environments for moderate to long periods of time will not occur (Jacobson and Smith 1990 as cited in ATSDR 1990).

3.0 FATE IN ECOLOGICAL RECEPTORS

Based on its short volatilization half life and low bioconcentration factor (Bysshe 1982; Hansch and Leo 1985), crotonaldehyde will not concentrate in aquatic organisms.

Little information was available on the fate of crontonaldehyde in mammals. Because crotonaldehyde has a low soil adsorption coefficient and strongly volatilizes, inhalation is the primary exposure route for mammals. Studies have indicated that inhaled crotonaldehyde is quickly absorbed by the upper and lower respiratory tracts (Egle 1972). Studies also suggest that absorbed crotonaledhyde is quickly metabolized (Alarcon 1976; Kaye 1973; Patel et al. 1980).

No information was available on the fate of crotonaldehyde in birds or plants.

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CUMENE (ISOPROPYLBENZENE)

1.0 SUMMARY

1-methylethylbenzene is also called cumene. Cumene and its superoxidized form, cumene hydroperoxide, are moderately volatile organic compounds. Cumene released to soil and surface water will rapidly dissipate through biodegradation and volatilization. Routes of exposure for cumene and cumene hydroperoxide include inhalation, ingestion, and dermal exposure. However, due to its high potential to volatilize, inhalation is the major exposure route for wildlife receptors. Bioconcentration of cumene is not likely in aquatic organisms. No information was available regarding the environmental fate of cumene hydroperoxide in air, water, or soil. However, degradation in soil and water is expected to be very rapid based on the high reactivity of cumene hydroperoxide with multivalent metal ions and free radicals.

The following is a profile of the fate of cumene and cumene hydroperoxide in soil, surface water and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, surface water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

The primary removal process for cumene in soil is expected to be through biodegradation in surface soil, and volatilization (HSDB 1997). Based on its log K_{oc} value (Lyman 1982), cumene that does not volatilize is expected to strongly adsorb to soil.

The environmental fate of cumene hydroperoxide in soil is unknown. However, based on its high reactivity with multivalent metal ions and free radicals, degradation in soil is expected to be very rapid (HSDB 1997).

In surface water, cumene is expected to have a relatively short half-life. The primary removal processes for cumene when released in water are volatilization and biodegradation (GEMS 1986; HSDB 1997). Based on different water characteristics, volatilization half-lives ranging from a few hours to a few days have been estimated (GEMS 1986). Cumene is amenable to biodegradation (Price et al. 1974; Kappeler and Wuhrmann 1978), and biodegrades in 10 to 30 days (Walker and Colwell 1975; Price et al. 1974).

The environmental fate of cumene hydroperoxide in water is unknown. However, based on its high reactivity with multivalent metal ions and free radicals, degradation in water is expected to be very rapid (HSDB 1997).

3.0 FATE IN ECOLOGICAL RECEPTORS

Cumene is reported to have relatively low bioconcentration in fish (ITC/EPA 1984; Geiger 1986;).

In wildlife, cumene and cumene hydroperoxide enter the body primarily via inhalation and dermal absorption (Lefaux 1968; HSDB 1997). Cumene is readily absorbed in mammalian systems and oxidized (Clayton and Clayton 1982). In the event that cumene is ingested, it is readily metabolized and excreted (Robinson et al. 1955). Long-term exposure by mammals results in cumene distribution to many tissues and organs (Gorban et al. 1978).

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DDE

1.0 SUMMARY

Dichlorodiphenyldichloroethane (DDE) is a high molecular weight, chlorinated pesticide. It is also a congener of dichlorodiphenyltrichloroethane (DDT), a full-spectrum pesticide. DDE is stable, accumulates in soil and sediment, and concentrates in fatty tissue. DDE has a low water solubility, and is adsorbed strongly in soils and sediments. Soil and benthic organisms accumulate DDE from soil and sediment. Wildlife will accumulate DDE in fatty tissue. Following chronic exposure by wildlife to DDE, an equilibrium between absorption and excretion may occur; however, concentrations will continue to increase because accumulation is related to fat content, which increases with age.

The following summarizes the fate of DDE in surface soil, surface water, and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, water, and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

DDE absorbs strongly to soil and is only slightly soluble in water. Under normal environmental conditions, DDE does not hydrolyze or biodegrade. In soils with low organic content, evaporation from the surface of soil may be significant (HSDB 1997).

DDE is bioavailable to plants and soil invertebrates despite being highly bound to soil. DDT has been found to accumulate in grain, maize, and rice plants with the majority located in the roots. Mobilization of soil-bound DDT by earthworms to more bioavailable forms has also been reported (Verma and Pillai 1991).

DDE is very persistent in the aquatic environment, has a very low water solubility, and is highly soluble in lipids. Compounds with these characteristics tend to partition to the organic carbon fraction of sediments and lipid fraction of biota (EPA 1986). DDE absorbs very strongly to sediment, and bioconcentrates in aquatic organisms (HSDB 1997). In aquatic environments, the small fraction of dissolved DDE may be photolyzed.

3.0 FATE IN ECOLOGICAL RECEPTORS

In general, DDE will bioconcentrate in lower-trophic-level organisms and will accumulate in food chains. Fish and other aquatic organisms readily take up pesticides, including DDE. Pesticides are taken up by organisms through the gills, by direct contact with the contaminant in the water, or by ingestion of contaminated food, sediment, or water. The lipophilic nature and extremely long half life of DDE result in bioaccumulation when it is present in ambient water. DDE will bioconcentrate in freshwater and marine plankton, insects, mollusks and other invertebrates, and fish (Oliver and Niimi 1985). When these organisms are consumed by other receptors, DDE is transferred up food chains. Following absorption, either through the gills or by ingestion, pesticides appear in the blood and may be distributed to tissues of all soft organs (Nimmo 1985).

DDE is accumulated to high concentrations in fatty tissues of carnivorous receptors. Elimination and absorption of DDE may occur simultaneously once an equilibrium is reached. This equilibrium may be disturbed by high concentrations of DDE, but termination of exposure usually results in elimination of the stored substance. This elimination occurs in two phases—an initial rapid phase followed by a much slower gradual loss (Nimmo 1985).

DDE can be introduced into mammals through oral, dermal, and inhalation exposure. Inhalation absorption is considered minor because the large particle size of DDE precludes entry to the deeper spaces of the lung; DDE is deposited in the upper respiratory tract and, through mucociliary action, is eventually swallowed and absorbed in the gastrointestinal tract. Gastrointestinal absorption following oral exposure has been shown in experimental animals (Hayes 1982). Dermal absorption is limited and the toxic effects are less than those seen following oral exposure. The highest concentration of DDE and metabolites has been found in adipose tissue, followed by reproductive organs, liver, kidneys, and brain (EPA 1980).

The metabolism of DDE in animals is similar to that in humans. DDE metabolism and elimination occurs very slowly. The primary route of elimination is in the urine (Gold and Brunk 1982, 1983, 1984); however, DDE may also be eliminated through the feces, semen, or breast milk. When exposure ceases, DDE is slowly eliminated from the body (Murphy 1986). The biological half-life of DDE is 8 years (NAS 1977).

Bioaccumulation has been reported in one Alaskan study of two raptor species—the Rough-legged hawk and the Peregrine falcon. Higher tissue residues were reported in the peregrine falcon than in the rough-legged hawk. It was believed that these differences may have been due to the different feeding habits of the birds (Matsumura 1985).

No information was available on the fate of DDE taken up by plants.

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DICHLOROFLUOROMETHANE

1.0 SUMMARY

Dichlorofluoromethane (DCFM) is a highly volatile hydrocarbon. It has a high vapor pressure and low soil adsorption coefficient; therefore, volatilization is the main fate process for DCFM released to surface soil and surface water. For terrestrial animals, inhalation is the main exposure route and ingestion is a minor exposure route. DCFM is not expected to bioconcentrate in fish; however, it can accumulate in tissues of mammals. DCFM is not expected to move up food chains.

The following information summarizes the fate of dichlorofluoromethane in soil, surface water and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

If released to soil, DCFM, an inert gas at room temperature, is expected to volatilize into the air due to its low soil adsorption coefficient (K_{oc}) value (Lyman et al. 1982). Because it does not have a strong affinity for organic carbon, it may dissolve in soil pore water, thus becoming bioavailable. Photooxidation, hydrolysis, and biodegradation are not likely to be significant removal processes for DCFM in soil due to its high volatility and minimal reactivity (HSDB 1997).

Based on its high water solubility and low soil adsorption coefficient, DCFM does not adsorb strongly to suspended solids or sediment. Based on a reported half-life of less than 1 day, DCFM is expected to rapidly volatilize from water (Lyman et al. 1982). The hydrolysis of DCFM is reported to be very low (<0.01 g/l of water-yr) (Du Pont de Nemours Co. 1980).

3.0 FATE IN ECOLOGICAL RECEPTORS

DCFM is not expected to bioconcentrate in aquatic organisms, based on its low log K_{ow} value (Hansch and Leo 1985) and low estimated BCF value (Lyman et al. 1982).

Information was not available on the fate of DCFM in mammals, birds, or plants.

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DICHLOROETHENE, 1,1-

1.0 SUMMARY

1,1-dichloroethene is a hydrophillic, low molecular weight, chlorinated hydrocarbon. It has a short half-life in the environment, thus acute exposures by ecological receptors are the main concern. Evaporation and biodegradation are major fate processes for 1,1-dichloroethene in soil, surface water, and sediment. It will also adsorb to detritus in soils and sediments. Ingestion and respiratory uptake are the significant direct exposure routes for ecological receptors exposed to 1,1-dichloroethene. Metabolic intermediates are responsible for the toxicity of 1,1-dichloroethene to upper trophic level receptors. Indirect (food chain) exposure through ingestion of contaminated food is minor because it is readily biotransformed and excreted. Hence, the biomagnification potential is very low.

The following is a profile of the fate of 1,1-dichloroethene in soil, surface water and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER AND SEDIMENT

If released onto the soil surface, the majority of 1,1-dichloroethene will quickly evaporate. Depending on the hydrogeology of a site, some may leach into ground water. Based on its high water solubility and small K_{oc} value, 1,1-dichloroethene may migrate through soils by adsorbing to dissolved organic carbon (EPA 1982). Studies have also documented that 1,1-dichloroethene will biodegrade in soils (HSDB 1997). A bioaccumulation factor for 1,1-dichloroethene in soil was not reported. However, based on its volatility and polarity, 1,1-dichloroethene is not expected to significantly bioaccumulate in soil (Callahan et al. 1979).

Evaporation is the major fate of 1,1-dichloroethene in surface water, with a short half-life of 1-6 days. Only a small quantity of 1,1-dichloroethene will be lost by adsorption onto the sediment (HSDB 1997). 1,1-dichloroethene also quickly biodegrades in aqueous environments. Degradation studies showed that 45–78% was lost in 7 days, when incubated with a wastewater inoculum. A large amount was also lost due to volatilization (Patterson and Kodukala 1981). In anaerobic environments, 1,1-dichloroethene

degrades (through reductive dechlorination) to vinyl chloride. Anaerobic degredation is slower that aerobic degradation. Approximately 50-80% of 1,1-dichloroethene underwent degradation in 6 months in a simulated groundwater environment (Barrio-Lage et al. 1986; Hallen et al. 1986). Photo-oxidation and hydrolysis are not expected to be significant removal processes for 1,1-dichloroethene (Callahan et al. 1979; Mabey et al. 1981; Cline and Delfino 1987). A bioaccumulation factor for 1,1-dichloroethene in water and sediment was not reported. However, based on its volatility and polarity, 1,1-dichloroethene is not expected to significantly bioaccumulate in water or sediment (Callahan et al. 1979).

3.0 FATE IN ECOLOGICAL RECEPTORS

Aquatic receptors may be directly exposed to dissolved 1,1-dichloroethene through gill respiration or through ingestion of suspended particles. Because 1,1-dichloroethene generally is not persistent in surface water, exposures are expected to be of short duration. 1,1-dichloroethene is not expected to bioconcentrate in fish or aquatic invertebrates, based on its low log K_{ow} value (Tute 1971; HSDB 1997). Due to limited bioconcentration, 1,1-dichloroethene is not expected to biomagnifiy in terrestrial or aquatic food chains (Barrio-Lage et al. 1986; Wilson et al. 1986).

1,1-dichloroethene is readily absorbed following inhalation (Dallas et al. 1983; McKenna et al. 1978a) or oral exposure, and is rapidly distributed in the body. Following inhalation exposure to 1,1-dichloroethene, uptake is dependent upon the duration of the exposure and the dose. Until equilibrium is reached, as exposure concentration increases, the percentage of 1,1-dichloroethene uptake decreases. Studies show that 2 minutes after inhalation exposure, substantial amounts of 1,1-dichloroethene were found in the venous blood of rats. Concentrations of 150 ppm or less of 1,1-dichloroethene showed a linear cumulative uptake. However, at 300 ppm steady state was not achieved, indicating saturation at high concentrations (Dallas et al. 1983).

Following oral administration of 1,1-dichloroethene in corn oil, rapid and almost complete absorption from the gastrointestinal tract of rats and mice was observed (Jones and Hathway 1978a; Putcha et al. 1986). Recovery of radio-labeled 1,1-dichloroethene was 43.55, 53.88, and 42.11%, 72 hours following oral administrations of 0.5, 5.0, and 50 mg/kg, respectively, to rats (Reichert et al. 1979). Also, 14.9-22.6% 1,1 dichloroethene was recovered in expired air, 42.11-53.88% in urine, 7.65-15.74% in feces, 2.77-5.57% in the carcass, and 5.91-9.8% in the cage rinse (Reichert et al. 1979).

1,1-dichloroethene is distributed mainly to the liver and kidneys following inhalation or oral exposure. In rodents, the highest levels of 1,1-dichloroethene are found in the liver and kidneys. Rats that were fasted and exposed to 1,1-dichloroethene showed significantly greater tissue burden than nonfasted rats (McKenna et al. 1978b; Jones and Hathway 1978b).

1,1-dichloroethene does not appear to be stored or accumulated in tissues, but is metabolized by the hepatic microsomal cytochrome P-450 system. This reaction produces reactive intermediates responsible for the toxicity of 1,1-dichloroethene. These reactive intermediates are detoxified through hydroxylation or conjugation with GSH, which is the primary biotransformation pathway in the rat. Excretion of unmetabolized 1,1-dichloroethene is through exhaled air, and metabolites are excreted via urine and exhaled air (Fielder et al. 1985; ATSDR 1994).

Avian receptors may be directly exposed to 1,1-dichloroethene through the ingestion of surface water and soil. Absorption studies specific to avian species were not identified in the literature.

Data on the fate of 1,1-dichloroethene in plant receptors were not identified in the literature. However, based on the low probability of significant bioaccumulation, uptake by plant receptors is expected to be minimal.

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DINITROTOLUENES

1.0 SUMMARY

2,4-dinitrotoluene and 2,6-dinitrotoluene are semi-volatile, nitrogen-substituted, organic compounds. They are moderately persistent in soil and have short half-lives in aqueous environments due to high rates of photolysis. Evidence also indicates that they are biodegraded in soil, surface waters and sediment. For wildlife, all routes of exposure are significant. Dinitrotoluenes are not expected to bioconcentrate in aquatic organisms and bioaccumulation is not expected in animal tissues. The major target organs following exposure to 2,4-dinitrotoluene are the liver and kidney. 2,6-dinitrotoluene is distributed to various organs following uptake. Evidence indicates that upper-trophic-level receptors rapidly metabolize 2,4-dinitrotoluene to innocuous by-products that are readily excreted. 2-6-dinitrotoluene is metabolized to a highly electrophilic ion that is capable of reacting with DNA and other biological nucleophiles.

The following summarizes the fate of 2,4-dinitrotoluene and 2,6-dinitrotoluene in soil, surface water and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

2,4-dinitrotoluene is expected to be slightly mobile in soil, based on its estimated K_{oc} value (Lyman et al 1982; Kenaga 1980). Information on the biodegradation of 2,4-dinitrotoluene in soil was not located; however, biodegradation is thought to occur in both aerobic and anaerobic zones of soil, based on aqueous biodegradation experiments (HSDB 1997).

2,6-dinitrotoluene readily biodegrades when released into the soil. Half-lives of 73 and 92 days were reported, when tested in two soils, with degradation rates of 0.5 to 0.7 mg/kg/day reported (Loehr 1989). Based on the calculated K_{oc} value (Lyman et al. 1982) and the estimated log K_{ow} value (GEMS 1984), 2,6-dinitrotoluene is expected to be slightly mobile in soil (Kenaga 1980).

Volatilization of dinitrotoluenes from surface soil is expected to be negligible due to very low vapor pressures of these compounds (Banerjee et al. 1990). Hydrolysis is not a significant removal process for nitroaromatic hydrocarbons (Lyman et al. 1982).

2,4-dinitrotoluene and 2,6-dinitrotoluene have a slight tendency to sorb to sediments, suspended solids, and biota, based on measured log K_{ow} values (GEMS 1984). In surface water, photolysis is the primary removal process for 2,4-dinitrotoluene and 2,6-dinitrotoluene. Reported half-lives range from a few minutes to a few hours (Spanggord et al. 1980; Zepp et al. 1984). Hydrolysis is not a removal process for nitroaromatics (Lyman et al. 1982).

Dinitrotoluenes do not readily volatilize in surface water. Volatilization half-lives of 2-4 dinitrotoluene from distilled water were 248 and 133 hours, which correspond to the volatilization rate constants of 0.0028 and 0.0052/hour (Smith et al. 1981). Davis et al. (1981), reported a 0.3 percent loss of 2,6-dinitrotoluene in a model waste stabilization pond. Empirical evidence indicates that dinitrotoluenes are expected to biodegrade in surface waters (Uchimura and Kido 1987; Umeda et al. 1985; Kondo et al. 1988; Tabak et al. 1981).

3.0 FATE IN ECOLOGICAL RECEPTORS

Aquatic organisms take up 2,4-dinitrotoluene, however, it does not bioconcentrate because it is readily eliminated. Measured BCF values for dinitrotoluenes are low indicating that bioconcentration does not occur in aquatic organisms (Deneer et al. 1987; EPA 1980).

Evidence indicates that once it is ingested by wildlife, 2,4-dinitrotoluene is rapidly absorbed into the bloodstream (Rickert et al. 1983). 2,4-dinitrotoluene is quickly distributed, with the highest concentrations in the liver and kidney (Rickert and Long 1981). The metabolism of 2,4-dinitrotoluene occurs in the liver and the intestine (via intestinal microflora), and it is quickly eliminated through the urine and feces (Lee et al. 1978; Long and Rickert 1982; Rickert and Long 1981; Schut et al. 1983). Based on the low log P value for 2,4-dinitrotoluene, bioaccumulation in animal tissues is not expected (Callahan et al. 1979; Mabey et al. 1981).

Dinitrotoluenes are expected to be readily taken up by plants, based on structural analogies with 1,3-dinitrobenzene and p-nitrotoluene (McFarlane et al. 1987; Nolt 1988).

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DI(N)OCTYLPHTHALATE

1.0 SUMMARY

Di(n)octylphthalate (DOP) is a high-molecular-weight, semi-volatile compound. It has a low water solubility and low vapor pressure, therefore it adsorbs strongly to the soil and sediment. Biodegradation is possible under aerobic conditions, but is slow under anaerobic conditions. DOP also undergoes hydrolysis in water. DOP may be absorbed following oral (dietary), inhalation, or dermal exposures, however dietary exposure is the most significant route of exposure. DOP may accumulate to increasing concentrations in algae, aquatic invertebrates, and fish, and accumulate to low levels in terrestrial wildlife. However, higher-trophic-level receptors will quickly metabolize it, therefore it does not biomagnify in food chains.

The following is a profile of the fate of DOP in soil, surface water and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER AND SEDIMENT

DOP has a very high K_{oc} value; therefore, it should adsorb strongly and remain immobile in soil (Wolf et al. 1980). Degradation in soil is slow, especially under anaerobic conditions (HSDB 1997).

Following release into aquatic environments, DOP adsorbs strongly to sediments and particulate material suspended in the water column (HSDB 1997). DOP has a moderate half-life in aquatic environments; losses are due to both volatilization and microbial degradation. Slow degradation is possible in aerobic conditions; however, DOP is resistant to anaerobic degradation (HSDB 1997). Approximately 50% degradation was observed within 5 days in a model terrestrial-aquatic ecosystem, with the monoester and phthalic acids the primary degradation products (Sanborn et al. 1975). DOP may bioconcentrate in aquatic organisms (Sanborn et al. 1975).

3.0 FATE IN ECOLOGICAL RECEPTORS

Sanborn et al. (1975) evaluated the bioconcentration and trophic transfer of DOP in model aquatic ecosystems containing phytoplankton, zooplankton, snails, insects, and fish. Evidence showed that the algae and invertebrates bioconcentrated DOP. Fish accumulated DOP to low levels, indicating that these receptors readily eliminate DOP.

DOP may be absorbed following oral, inhalation or dermal exposures (EPA 1980a); however, due to low volatility of DOP, inhalation is not a significant route of exposure (Meditext 1997). Following absorption, DOP is rapidly distributed with the highest amounts concentrated in the liver, kidney and bile (EPA 1980b). DOP is rapidly metabolized to water-soluble derivatives (Gosselin et al. 1984) prior to and after absorption (EPA 1980b). These metabolites are then excreted through the urine and the bile (Ikeda et al. 1978).

No information was available on the fate of DOP in birds or plants.

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DIOXANE, 1,4-

1.0 SUMMARY

1,4-dioxane is a highly water-soluble, moderately volatile organic compound. In soil, surface water, and sediment environments, 1,4-dioxane is not persistent because it is volatile and because it has a low affinity for adsorption to organic carbon. It has a low potential to bioconcentrate in aquatic receptors. Wildlife can be exposed to 1,4-dioxane through ingestion, inhalation, and dermal contact. It does not bioaccumulate in food chains.

The following is a profile of the fate of 1,4-dioxane in soil, surface water and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER AND SEDIMENT

Based on an estimated log K_{oc} value (Lyman et al. 1982), 1,4-dioxane is expected to have a low affinity for organic carbon in soil, thus having a high potential to leach out of surface soils (HSDB 1997). This reduces the exposure potential for vegetation (through root uptake) and soil invertebrates. In addition, because of its moderate vapor pressure, volatilization is expected to be a significant fate process in soil (Verschueren 1983). Based on the volatility of 1,4-dioxane, biaccumulation is not considered to be a significant fate process in soil.

1,4-dioxane is infinitely soluble in water (Lange 1967). However, because 1,4-dioxane has a moderate vapor pressure at 25°C, volatilazation from water is a significant removal process (Verschueren 1983; HSDB 1997). 1,4-dioxane is not expected to adsorb to suspended sediments or detritus due to the estimated K_{oc} value (HSDB 1997). Based on its high volatility in water and low absorption to sediments, bioaccumulation is not expected to be a significant fate process for 1,4-dioxane in water and sediment.

3.0 FATE IN ECOLOGICAL RECEPTORS

Because it is highly soluble in water, aquatic receptors can take up 1,4-dioxane through direct exposure, however, it is not expected to bioconcentrate based on its low K_{ow} value (Hansch and Leo 1985).

Information suggests that 1,4-dioxane has a low potential to be biodegraded in aerobic aquatic environments. Biodegradation experiments with activated sludge showed a negligible biochemical oxygen demand for 1,4-dioxane, therefore, classifying 1,4-dioxane as relatively undegradable (Mills 1954; Alexander 1973; Heukelekian and Rand 1955; Fincher and Payne 1962; Lyman et al. 1982; Kawasaki 1980).

No information was available on the fate of 1,4-dioxane after uptake by aquatic receptors. However, its low bioconcentration factor suggests that 1,4-dioxane is readily eliminated after uptake (Hansch 1985).

The metabolism of 1,4-dioxane in rats has been studied, and information indicates that at high daily doses, 1,4-dioxane can induce its own metabolism. There is an apparent threshold of toxic effects of 1,4-dioxane that coincides with saturation of the metabolic pathway for its detoxification (Young et al. 1978). 1,4-dioxane is highly toxic via all routes of exposure (OHM/TADS 1997), and is readily absorbed through intact skin (Gosselin 1984). Once 1,4-dioxane enters the body, it is distributed throughout the tissues, including the liver, kidney, spleen, lung, colon, and skeletal muscle (Woo et al. 1977). The excretion of 1,4-dioxane is primarily through the urine, in which approximately 85% of excreted material is in the form of beta-hydroxyethoxyacetic acid, a metabolic byproduct. The remaining material is excreted as unchanged dioxane (Braun & Young 1977).

Information was not available on the fate of 1,4-dioxane in birds or plants.

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DIBENZO-*p*-DIOXINS

1.0 SUMMARY

Dibenzo-p-dioxins (dioxins) are a group of high molecular weight chlorinated compounds that are highly soluble in fatty tissues. The congener tetrachlorodibenzodioxin (TCDD) is commonly used as a surrogate for estimating the fate of dioxins in the environment and in ecological receptors. Dioxins have low water solubilities and adsorb strongly to organic carbon in sediment and soil. Dioxins bioaccumulate in aquatic organisms and wildlife, and biomagnify in food chains because of their affinity for lipids. Biomagnification of TCDD appears to be significant between fish and fish-eating birds, but not between fish and their food (other fish).

The following is a profile of the fate of dioxins in soil, surface water, and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, water, and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

TCDD adsorbs strongly to soils (HSDB 1997). TCDD in soil may be susceptible to photodegradation. Volatilization from soil surfaces during warm months may be a major mechanism by which TCDD is removed from soil. Various biological screening studies have demonstrated that TCDD is generally resistant to biodegradation. The half-life of TCDD in surface soil varies from less than 1 year to 3 years. Half-lives in deeper soils may be as long as 12 years (EPA 1993).

TCDD is very persistent in the aquatic environment, has a very low aqueous solubility, and is highly soluble in lipids. Aquatic sediments are an important reservoir for dioxins, and may be the ultimate environmental sink for all global releases of TCDD (HSDB 1997). TCDD may be removed from water through either photolysis or volatilization. The photolysis half-life at surface level has been estimated to range from 21 hours in summer to 118 hours in winter (HSDB 1997). These rates increase significantly with increasing water depths. Therefore, many bottom sediments may not be susceptible to significant photodegradation. The volatilization half-life from the water column of an environmental pond has been estimated to be 46 days, and may be as high as 50 years if adjusted for the effects of sediment adsorption.

Various biological screening studies have demonstrated that TCDD is generally resistant to biodegradation. The persistent half-life of TCDD in lakes has been estimated to be in excess of 1.5 years (HSDB 1997).

3.0 FATE IN ECOLOGICAL RECEPTORS

Ecological exposures to TCDD can occur via ingestion of contaminated soils, water, and sediment, dermal exposure to soil and water, and to a much lesser extent via inhalation of airborne vapors and particulates. It should be noted that, unlike toxicokinetic and toxicodynamic studies where exposures are closely controlled, environmental exposure to dioxin occurs as a complex mixture of congeners, including TCDD. It is generally understood that persistent, lipophilic compounds accumulate in fish in proportion to the lipid content and age of each animal (Gutenmann et al. 1992). Also, it has been demonstrated that the influence of biotransformation on bioaccumulation increases as a function of the K_{ow} of the compound (de Wolf et al. 1992). The dependence of metabolic rate on TCDD dose and length of exposure is not well understood, but time-course studies of P-450 induction in rainbow trout by β-napthoflavone demonstrate that different toxicity responses can occur over time depending on the frequency and duration of exposure (Zhang et al. 1990).

Dioxins readily bioconcentrate in aquatic organisms (Branson et al. 1985; Mehrle et al. 1988; Cook et al. 1991; and Schmieder et al. 1992). Evidence indicates that dioxins will distribute in fish tissues in proportion to the total lipid content of the tissues (Cook et al 1993). Dioxins are metabolized and eliminated very slowly from fish (Kleeman et al. 1986a,b; Opperhuizen and Sijm 1990; Kuehl et al. 1987).

Several studies in a wide range of mammalian and aquatic species indicate that TCDD is metabolized to more polar metabolites (Ramsey et al. 1979; Poiger and Schlatter 1979; Olson et al. 1980; Olson 1986; Poiger et al. 1982; Sijm et al. 1990; Kleeman et al. 1986a,b, 1988; Gasiewicz et al. 1983; Ramsey et al. 1982). The metabolism of TCDD and related compounds is required for urinary and biliary elimination and plays an important role in regulating the rate of excretion of these compounds.

Dioxins are transferred through food chains, biomagnifying in upper-trophic-level receptors, especially birds. Biomagnification of TCDD appears to be significant between fish and fish-eating birds but not between fish and their food (Carey et al. 1990). The lack of apparent biomagnification between fish and their prey is probably due to the influence of biotransformation of TCDD by the fish. Limited data for the

base of the Lake Ontario lake trout food chain indicates little or no biomagnification between zooplankton and forage fish (Whittle et al. 1992). BMFs based on fish consuming invertebrate species probably are close to 1.0 because of the TCDD biotransformation by forage fish.

Oral absorption of dioxin related compounds in laboratory animals has been reported to be contingent on species, test compound, administered dose, and vehicle. Typical oral absorption values range from 50 to 90 percent (EPA 1994). Because TCDD in the environment is likely to be adsorbed strongly to soil, the oral bioavailability of TCDD varies significantly from laboratory values. Studies have shown that oral bioavailability of TCDD in soil is lower by as much as 50 percent as compared to oral bioavailability of TCDD administered in corn oil over a 500-fold dose range (EPA 1994). Moreover, oral bioavailability of TCDD may be significantly lower in different soil types, with values as low as 0.5 percent bioavailability reported (Umbreit et al. 1986 a,b).

Dermal absorption of TCDD has been studied extensively in laboratory animals. Dermal absorption has been demonstrated to depend on applied dose, with lower relative absorption (percentage of administered dose) decreasing at higher doses (Brewster et al. 1989). Dermal absorption rates in laboratory rats ranged from 17 to 40 percent of administered dose (Brewster et al. 1989). Percent bioavailability of TCDD following dermal absorption is significantly lower than bioavailability following oral absorption by as much as 60 percent (Poiger and Schlatter 1980). As with oral absorption of TCDD in soil, percent bioavailability following dermal exposure to TCDD in soil was significantly lower than percent bioavailability following an equivalent oral dose (approximately 1 percent of an administered dose) (Shu et al. 1988).

Transpulmonary absorption of TCDD has been studied in laboratory animals following intratracheal instillation of the compound in various vehicles (Nessel et al. 1990, 1992). Systemic effects characteristic of TCDD exposures, including hepatic microsomal cytochrome p-450 induction, were observed after inhalation exposures, indicating that transpulmonary absorption does occur and that inhalation may be an important route of TCDD exposure. Transpulmonary bioavailability was estimated at approximately 92 percent of administered dose, very similar to that observed after oral exposures (Diliberto et al. 1992). It should be noted that in an environmental setting, inhalation exposures to TCDD in fly ash, dust and soil particulates may be associated with very different absorption and bioavailability patterns.

Tissue distribution studies in laboratory rats and mice indicate that TCDD is distributed preferentially to adipose tissue and liver (EPA 1994). TCDD is distributed to other organs as well, but to a lesser extent. Also, tissue distribution of TCDD has been demonstrated to be time and dose-dependent, with increasing levels of TCDD distributing to adipose and liver associated with higher doses and increased latency period from time of dosage (EPA 1994).

Plants will take up TCDD through root uptake from soil and through foliar uptake from air (EPA 1994). No other information was available on the fate of dioxins after uptake by plants.

No information was available on the fate of dioxins in birds.

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DIBENZOFURANS

1.0 SUMMARY

Polychlorinated dibenzofurans (PCDF) are a class of hydrophobic chlorinated compounds that adsorb strongly to soils and sediments. Like dioxins, PCDFs are persistent in the environment, bioconcentrate in aquatic organisms, and biomagnify in some food chains. Because PCDFs are associated with organic material in abiotic media, direct contact by soil and sediment receptors, and ingestion by bottom-feeding fish and upper trophic level wildlife, are the most important exposure routes.

Since PCDFs are structurally similar to, and behave in the environment like dioxins, fate of PCDFs is inferred from information about dioxins. Most of the description on the fate of PCDFs is based on the behavior of tetrachlorodibenzofuran (TCDF), one of the most toxic PCDF congeners. The following is a profile of the fate of polychlorinated dibenzofurans (PCDFs) in soil, water, and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, surface water, and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

TCDF adsorbs strongly to soils. Based upon its high K_{oc} value, TCDF is expected to sorb very strongly in soil and not be susceptible to leaching under most soil conditions. No data are available regarding the biological degradation of TCDF in soil (HSDB 1997).

TCDF in the water column can be expected to partition strongly to sediment and suspended particulate matter. Volatilization from the water column can be important, however the significance of this fate process is limited by strong sorption to sediments (HSDB 1997). Bioconcentration in aquatic organisms may be significant. Aquatic hydrolysis is not expected to be important. Data on biodegradation of TCDF are unavailable (HSDB 1997).

3.0 FATE IN ECOLOGICAL RECEPTORS

Based on high Kow values, PCDFs are expected to accumulate in aquatic receptors (Gutenmann et al. 1992).

Based on its similar structure to dioxins, PCDFs are expected to accumulate to high concentrations in aquatic and semi-aquatic mammals and in fish-eating birds.

Information was not available on the disposition of PCDFs in plants.

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HEXACHLOROBENZENE

1.0 SUMMARY

Hexachlorobenzene (HCB) is a persistent chemical that adsorbs strongly to soil and sediment. It is relatively stable in the environment and is resistant to hydrolysis, photolysis, and oxidation, with relatively no metabolism by microorganisms. Due to its high affinity for organic carbon, HCB will accumulate in sediments. Soil invertebrates and benthic invertebrates will take up HCB directly from these media. For higher-trophic-level receptors, indirect (food chain) exposure is anticipated to be the most significant pathway because HCB is resistant to metabolism and is very soluble in fat. The major toxic effect that has been observed across all species tested is porphyria.

The following is a profile of the fate of HCB in soil, surface water and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

Due to a long half-live in soil and its strong affinity for organic carbon, HCB released to soil is likely to remain there for extended periods of time (Beck and Hansen 1974). Minimal biodegradation occurs, depending on the organic carbon content of the soil. Some evaporation from surface soil to air may occur, again depending on the organic carbon content of the soil (Gile and Gillett 1979).

Once released to water, HCB will either evaporate rapidly or adsorb to sediments, with very little dissolved in water (HSDB 1997; Kelly et al. 1991). Limited degradation of HCB is expected, since it appears to be stable to hydrolysis, photolysis, and oxidation (Callahan et al. 1979). Since HCB adsorbs strongly to sediments, it may build up in bottom sediments.

3.0 FATE IN ECOLOGICAL RECEPTORS

Aquatic organisms may be exposed to HCB through ingestion of contaminated water, soil, sediment, or food. Empirical information indicates that HCB bioconcentrates in fish and invertebrates (Giam et al.

1980; Konemann and Vanleeuwen 1980; Veith et al. 1979; Oliver and Niimi 1983; Parrish et al. 1978; Kosian et al. 1978; Neely et al. 1974; Zitko and Hutzinger 1976; Laseter et al. 1976).

HCB can be transferred through aquatic food chains. Knezovich and Harrison (1988) reported that chironomid larvae, a common food item of young fish and other aquatic receptors, rapidly bioaccumulate HCB and other chlorobenzenes from contaminated sediments, achieving steady state within 48 hours. Information was not available about metabolism of HCB by fish.

Ingestion of contaminated media and food is the main route of mammalian exposure to HCB (HSDB 1997; ATSDR 1994; Edwards et al. 1991). Following ingestion, HCB is readily absorbed and is distributed through the lymphatic system to all tissues. It accumulates in fatty tissues and persists for many years since it is highly lipophilic and is very slowly metabolized (Weisenberg 1986; Mathews 1986).

HCB is slowly metabolized by the hepatic cytochrome P-450 system, conjugated with glutathione, or reductively dechlorinated (ATSDR 1994). The metabolites of HCB in laboratory animals include pentachlorophenol, pentachlorobenzene, tetrachlorobenzene, traces of trichlorophenol, a number of sulfur containing compounds, and some unidentified compounds (Mehendale et al. 1975; Renner and Schuster 1977, 1978; Renner et al. 1978; Edwards et al. 1991).

Plants take up relatively minimal amounts of HCB from soils (EPA 1985; Carey et al. 1979). Information was not available on the fate of HCB in birds.

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HEXACHLOROBUTADIENE

1.0 SUMMARY

Hexachlorobutadiene (HCBD) is a moderately volatile, high molecular weight, chlorinated compound. In surface soil and sediment, it will adsorb to organic carbon. It is moderately soluble in water. In surface water, it will adsorb to suspended material; however, it has a tendency to volatilize. In aerobic environments, in will biodegrade. Exposure routes for aquatic organisms include ingestion, gill uptake, and dermal contact. HCBD bioconcentrates in aquatic life. For mammalian and avian wildlife, HCBD can be taken up through oral, inhalation, and dermal exposure routes. HCBD is not expected to bioaccumulate to high levels in upper-trophic-level receptors. HCBD metabolites cause adverse effects.

The following is a profile of the fate of HCBD in soil, surface water and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

HCBD has a high soil partition coefficient, and would, therefore, be expected to adsorb to soils with a high organic content (Montgomery and Welkom 1990); however, in sandy soils with a low organic content, HCBD is more mobile and will be found in soil pore water (Piet and Zoeteman 1980). HCBD also has a moderate potential to evaporate from surface soils, unless it is bound to organic carbon (Pearson and McConnel 1975). HCBD is expected to biodegrade in aerobic soils (Tabak et al. 1981), but not in anaerobic environments (Johnson and Young 1983).

Following release into water, HCBD will either quickly volatilize or adsorb to sediments and suspended material (Montgomery and Welkom 1990). HCBD will accumulate concentrations in sediments (Elder et al. 1981; EPA 1976; Oliver and Charlton 1984). Biodegradation is a significant removal process for HCBD in aerobic environments (Tabak et al. 1981). However, under anaerobic conditions biodegradation does not occur (Johnson and Young 1983).

3.0 FATE IN ECOLOGICAL RECEPTORS

HCBD dissolved in surface water is expected to bioconcentrate in aquatic organisms, including algae, benthic macroinvertebrates (such as worms and bivalves), detritivore (crayfish), and plantivorous fish (EPA 1976, Oliver and Niimi 1983). HCBD also accumulates in carnivorous fish (EPA 1976). In fish, HCBD will distribute to fatty tissue, especially the liver (Pearson and McConnell 1975 as cited in ATSDR 1994).

Mammals may be exposed to HCBD through (1) ingestion of soil and exposed sediment while foraging for food, grooming, and soil covering plant matter, (2) ingestion of drinking water, and (3) indirect ingestion of contaminated plant and animal matter. Based on HCBD's affinity for soil and sediment, and its potential to be bioconcentrated, it is anticipated that indirect exposure will be the most significant exposure route for mammals. Once ingested, HCBD is readily absorbed in the gastrointestinal tract (Reichert et al. 1985). Following absorption, HCBD is distributed primarily to the kidney, liver, adipose tissue, and brain (Dekant et al. 1988; Nash et al. 1984; Reichert et al. 1985).

HCBD does not appear to be metabolized by the hepatic mixed function oxidase system; however, it does undergo conjugation with glutathione in the liver (Garle and Fry 1989). Metabolic derivatives of these conjugates are believed to be responsible for the renal damage associated with exposure to HCBD (Dekant et al. 1991; Koob and Dekant 1992).

In gravid birds, low levels of HCBD will be transferred to eggs (Dow Chemical Co. 1972).

Information was not available on the fate of HCBD in plants.

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HEXACHLOROCYCLOPENTADIENE

1.0 SUMMARY

Hexachlorocyclopentadiene (HCCP) is a semi-volatile, chlorinated compound. If HCCP is released as an emission product, it has been shown to exist mostly in the vapor phase, with photolysis resulting in rapid degradation. HCCP in soil will adsorb to soil particles. Degradation of HCCP may also occur in the environment by chemical hydrolysis and biodegradation by soil biota. Depending on the route of exposure, HCCP may distribute mainly to the lungs, kidneys, and liver. HCCP could potentially bioaccumulate in some aquatic organisms depending upon the species. The respiratory system is the major site of toxicity following inhalation exposure, while, depending on the species, the kidney or the liver are the major sites of toxicity following oral exposure.

The following is a profile of the fate of HCCP in soil, surface water and sediment, and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

HCCP deposited to soil is expected to adsorb strongly to organic carbon in the soil (HSDB 1997). Volatilization from soil surfaces is expected to be minor. In moist soil, hydrolysis and biodegradation under aerobic and anaerobic conditions may occur (HSDB 1997). HCCP on the surface of soil may be subject to photolysis.

HCCP present in surface water will degrade primarily by photolysis and chemical hydrolysis. The half-life of HCCP from photodegradation is very short ; Wolfe et al.(1982) reported a half-life of less than 15 minutes in the top of the water column. In unlit or deep, turbid water, the degradation of HCCP occurs by chemical hydrolysis. Hydrolytic half-lives for HCCP range from several hours to 2-3 weeks, depending on the temperature of the water (Chou et al. 1981; Zepp and Wolfe 1987). HCCP has the potential to adsorb to suspended solids in surface water and sediments; however, this adsorption does not affect the rate of hydrolysis (Wolfe et al. 1982).

Volatilization from water is also expected to be a significant removal mechanism; however, adsorption to suspended solids and sediments may interfere with this process. (EPA 1987).

3.0 FATE IN ECOLOGICAL RECEPTORS

HCCP is expected to be moderately bioconcentrated by algae, invertebrates, and fish. (Lu et al. 1975; Spehar et al. 1979; Veith et al. 1979; Podowski and Khan 1984; Freitag et al. 1982) (Geyer et al. 1981). HCCP taken up by freshwater fish (goldfish) is readily distributed, stored, and metabolized (Podowski et al. 1991). In fish, HCCP is excreted in the bile. The biological half-life of HCCP in the goldfish was approximately 9 days (Podowski and Khan 1984).

Inhalation is the main exposure route for HCCP toxicity in mammals. HCCP is less absorbed following ingestion (Lawrence and Dorough 1981). Following ingestion, HCCP will move primarily to the liver and the kidney (Lawrence and Dorough 1981), which appear to be the main sites of toxicity (Abdo et al. 1984; Southern Research Inst 1981).

Limited information was available regarding the metabolism of HCCP. Some degradation may occur in the gut following oral administration (Dorough and Ranieri 1984; Mehendale 1977).

Information was not available on the fate of HCCP in birds or plants.

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HEXACHLOROPHENE

1.0 SUMMARY

Hexachlorophene is a persistent organic chemical that is highly soluble in lipids and adsorbs strongly to soil and sediment In surface soils and the euphotic (light-penetrating) zone of surface waters, hexachlorophene is degraded by photolysis. Hexachlorophene may be bioconcentrated by aquatic and soil organisms. In upper-trophic-level receptors, hexachlorophene may be absorbed following oral or dermal exposure and is distributed throughout all body tissues. Due to its high lipid solubility, hexachlorophene has the potential to be transferred significantly in food chains. In mammals, the nervous system is the major site of toxicity for hexachlorophene; however, reproductive and developmental effects have also been reported. Exposure to hexachlorophene may result in decreased egg production in birds.

The following is a profile of the fate of hexachlorophene in soil, surface water, and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, water, and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

Hexachlorophene adsorbs strongly to soil and once bound does not tend to leach from soil or mobilize in soil. Hexachlorophene does not undergo significant hydrolysis or evaporation from the soil; however, slow photodegradation may occur if exposed to light above 290 nm (Kotzias et al. 1982).

Hexachlorophene does not undergo hydrolysis, evaporation or volatilization in water; however, slow photodegradation may occur. Hexachlorophene adsorbs strongly to sediments and has been identified in the humic acid portion of sediment. The half-life of hexachlorophene in water is expected to be greater than 50 years with a half-life of 290 days reported in sediment. Hexachlorophene has been reported to bioconcentrate in aquatic organisms (Kotzias et al. 1982; Hansch and Leo 1985; Lyman et al. 1982).

3.0 FATE IN ECOLOGICAL RECEPTORS

Based on its high octanol-water partition coefficient, hexachlorophene is expected to bioconcentrate in aquatic life living in the water column and in the sediment. Bioconcentration has been measured in mosquito fish and snail (Hansch and Leo 1985; Lyman et al. 1982).

Hexachlorophene is absorbed rapidly following oral exposure (Hatch 1982). Hexachlorophene may also be absorbed following dermal exposure with blood levels peaking approximately 6 to 10 hours post-application (Meditext 1997). Hexachlorophene is highly lipid-soluble. After entering the bloodstream, it distributes into adipose tissue and tissue with a high lipid content including the central nervous system. Hexachlorophene binds preferentially to myelin (Meditext 1997). Transplacental transfer of hexachlorophene has also been reported (Hatch 1982). Target organs include the nervous system, the gastrointestinal system, and skin (Meditext 1997).

Hexachlorophene has been reported to have low volatility from plant leaves (Goetchius et al. 1986). Additional data regarding the potential effects of hexachlorophene on plants were not located. Information was not available on the fate of hexachlorophene in exposed birds.

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HYDRAZINE

1.0 SUMMARY

Hydrazine is a reactive, nitrogen-containing compound. It is readily biodegraded after release to soil and surface water. Volatilization may also be a significant removal process. Hydrazine is readily absorbed following inhalation, ingestion, and dermal absorption. Mammals rapidly break down and excrete hydrazine.

The following is a profile of the fate of hydrazine in soil, surface water and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, surface water, and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

Studies show that hydrazine is expected to biodegrade in soils high in organic carbon, and to adsorb to soils high in clay content (Braun and Zirrolli 1983; Sun et al. 1992). For dry surface soil, volatilization may be a significant process (HSDB 1997).

Hydrazine is expected to have a relatively short half-life of 8.3 days in pond water (Braun and Zirrolli 1983). Hydrazine has been reported to react with dissolved oxygen at a rate inversely proportional to its concentration (Slonim and Gisclard 1976); its degradation rate increases with increasing temperature, dissolved oxygen, and the presence of microorganisms (Sun et al. 1992).

3.0 FATE IN ECOLOGICAL RECEPTORS

Hydrazine is absorbed rapidly from the lungs, gastrointestinal tract, and through skin (ACGIH 1991). Hydrazine is reported to be neurotoxic, hepatotoxic and nephrotoxic in rodents (Lambelt and Shank 1988). Hydrazine is rapidly metabolized in the liver and eliminated (Jenner and Timbrell 1995).

Information was not available on the fate of hydrazine in exposed birds, aquatic life, or plants.

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MERCURY

1.0 SUMMARY

Mercury is a highly toxic compound with no known natural biological function. Mercury exists in three valence states: mercuric (Hg2+), mercurous (Hg1+), and elemental (Hg0+) mercury. It is present in the environment in inorganic and organic forms. Inorganic mercury compounds are less toxic than organomercury compounds, however, the inorganic forms are readily converted to organic forms by bacteria commonly present in the environment. The organomercury compound of greatest concern is methylmercury.

Mercury sorbs strongly to soil and sediment. Elemental mercury is highly volatile. In aquatic organisms, mercury is primarily absorbed through the gills. In aquatic and terrestrial receptors, some forms of mercury, especially organomercury compounds, bioaccumulate significantly and biomagnify in the food chain. In all receptors, the target organs are the kidney and central nervous system. However, mercury causes numerous other effects including teratogenicity and mutagenicity.

The following is a profile of the fate of mercury in soil, surface water and sediment, and the fate after uptake by biological receptors. Section 2 discusses the environmental fate and transport in soil, surface water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

In soil, mercury exists in the mercuric (Hg2+) and mercurous (Hg1+) states. Mercury adsorbs to soil or is converted to volatile forms (Krabbenhoft and Babiarz 1992; Callahan et al. 1979). Mercury can migrate by volatilization from aquatic and terrestrial sources through the reduction of metallic mercury to complex species and by the deposition in reducing sediments. Atmospheric transport is a major environmental distribution pathway.

Mercury 2+ is the predominant form of mercury in surface waters (ATSDR 1993). Nonvolatile mercury in surface water binds to organic matter and sediment particles (Lee and Iverfeldt 1991).

Sorption to suspended and bed sediments is one of the most important processes determining the fate of mercury in aquatic systems; sorption onto organic materials is the strongest for mercury 2+. As a result, mercury is generally complexed to organic compounds and is not readily leached from either organic-rich or mineral-rich soils (Rosenblatt et al 1975). Most mercury compounds can be remobilized in aquatic systems by microbial conversion to methyl and dimethyl forms. Conditions reported to enhance microbial conversion include large amounts of available mercury, large numbers of bacteria, absence of strong complexing agents, near neutral pH, high temperatures, and moderately aerobic conditions.

3.0 ECOLOGICAL RECEPTORS

Sorption at the gill surface is the major pathway of mercury entry in aquatic organisms (EPA 1984). In aquatic organisms, bioaccumulation is rapid and elimination is slow. Biomagnification occurs in the aquatic food chain (NRCC 1979). Absorbed mercury is distributed to the blood and ultimately the internal organs. Mercury which is not absorbed is eliminated rapidly in the feces (Eisler 1987). The biological half-life of mercury in fish is approximately 2 to 3 years (EPA 1985). In general, mercury accumulation is enhanced by elevated water temperatures, reduced water hardness or salinity, reduced water pH, increased age of the organism, reduced organic matter content of the medium, and the presence of zinc, cadmium, or selenium in solution.

Mercury is readily absorbed by terrestrial species following oral and inhalation exposure. Elemental and organomercury compounds are readily transferred across the placenta and blood-brain barrier. Mercury is bioaccumulated primarily in the kidney (Rothstein and Hayes 1964; Nielsen and Andersen 1991), and mercury is biomagnified in mammals (Eisler 1987). Retention of mercury in mammals is longer for organomercury compounds (especially methylmercury) than for inorganic forms. Mercury elimination occurs via the urine, feces, expired air, and breast milk (Clarkson 1989; Yoshida et al. 1992).

All mercury compounds interfere with metabolism in organisms, causing inhibition or inactivation of proteins containing thiol ligands and ultimately leading to miotic disturbances (Das et al 1982; Elhassani 1983). Mercury also binds strongly with sulfhydryl groups. Phenyl and methyl mercury compounds are among the strongest known inhibitors of cell division (Birge et al 1979). In mammals, methyl mercury irreversibly destroys the neurons of the central nervous system.

Information was not available on the fate of mercury in birds.

Mercury in soils is generally not available for uptake by plants due to the high binding capacity to clays and other charged particles (Beauford et al 1977). However, mercury levels in plant tissues increase as soil levels increase with 95% of the accumulation and retention in the root system (Beauford et al 1977; Cocking et al 1991). Mercury is reported to inhibit protein synthesis in plant leaves and may affect water-adsorbing and transporting mechanisms in plants (Adriano 1986).

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METHANOL

1.0 SUMMARY

Methanol is a highly water soluble hydrocarbon. It does not adsorb to organic carbon. The primary removal process for methanol in soil and water is biodegradation. Aquatic, soil, and sediment communities can be exposed to methanol through direct contact. Upper-trophic-level receptors may be directly exposed through ingestion, inhalation, or dermal exposure. Methanol does not bioconcentrate or move through food chains.

The following is a profile of the fate of methanol in soil, surface water, and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, surface water, and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

Based on biological screening studies, including soil microcosm studies, methanol undergoes biodegradation if released to the soil. Methanol is expected to be highly mobile in soil, based on its miscibility in water and low log K_{ow} value. Evaporation from dry surfaces is also expected to occur, based on the high vapor pressure of methanol (Weber et al. 1981; Hansch and Leo 1985; HSDB 1997).

Methanol is completely soluble in water. Methanol is significantly biodegradable in water, based on screening studies (HSDB 1997). Volatilization is expected to be a significant removal process (Lyman 1982). Aquatic hydrolysis, oxidation, photolysis, adsorption to sediment, and bioconcentration are not considered significant removal processes for methanol (HSDB 1997).

3.0 FATE IN ECOLOGICAL RECEPTORS

Methanol uptake across gill epithelia is the most significant exposure route. However, based on its low bioconcentration factor for fish, methanol does not bioconcentrate (Freitag et al. 1985; Bysshe 1982) (Hansch and Leo 1985).

Mammals are exposed to methanol through ingestion, inhalation, and dermal contact. Methanol is reported to readily absorb from the gastrointestinal and respiratory tracts (Gosselin et al. 1984), and rapidly distribute within tissues (Clayton and Clayton 1982). Following absorption, methanol is widely distributed in body tissue. Small amounts are excreted in the urine and expired air; however, methanol is mostly oxidized to formaldehyde and formic acid (Goodman and Gillman 1985).

Information was not available on the fate of methanol in exposed birds or plants.

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NITROPROPANE, 2-

1.0 SUMMARY

2-nitropropane is a highly volatile, low molecular weight hydrocarbon. Generally, it does not adsorb to soil or sediment, and rapidly volatilizes from soil and surface water. Wildlife may be exposed to 2-nitropropane through ingestion or inhalation. Due to its high water solubility, 2-nitropropane does not bioconcentrate in fish, and does not bioaccumulate in wildlife. 2-nitropropane is rapidly metabolized and excreted by mammals.

The following summarizes information on the fate of 2-nitropropane in soil, surface water and sediment, and its fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

2-nitropropane rapidly volatilizes from soil, and also has the potential to leach in moist soils. 2-nitropropane undergoes minimal degradation in soil (Freitag et al. 1988).

2-nitropropane is highly soluble in water (Baker and Bollmeier 1981). It is expected to have a short half-life in surface water because of its propensity for rapid volatilization, based on its high vapor pressure (Dougan et al. 1976). Adsorption of 2-nitropropane to suspended solids or sediment is not expected, based on its low K_{oc} value (Lyman 1982).

3.0 FATE IN ECOLOGICAL RECEPTORS

2-nitropropane does not bioconcentrate in aquatic organisms (Baker and Bollmeier 1981; Freitag et al. 1988). 2-nitropropane is readily absorbed by the gastrointestinal tract and the lungs, when inhaled. Accumulation of 2-nitropropane in tissues of mammals is low because it is rapidly metabolized and eliminated after uptake (Nolan et al. 1982). 2-nitropropane may be excreted unchanged in expired air or as nitrite and nitrate in the urine (Browning 1965).

No information was available on the fate of 2-nitropropane in birds or plants.

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POLYNUCLEAR AROMATIC HYDROCARBONS (PAHS)

1.0 SUMMARY

Polynuclear aromatic hydrocarbons (PAH) are a class of semi-volatile compounds that have a high affinity for soil and sediment particles. PAHs have low water solubility. Low molecular weight PAHs volatilize and photolyze from soil and surface water, and may be biodegraded as well. High molecular weight PAHs are resistant to volatilization, photolysis, and biodegradation. PAHs can be bioconcentrated to high concentrations by some aquatic organisms. However, many aquatic organisms can metabolize PAHs. The main PAH exposure route for upper-trophic-level receptors is ingestion. However, wildlife can readily metabolize PAHs and eliminate the by-products. Therefore, food chain transfer and biomagnification are anticipated to be minimal.

The following is a profile of the fate of PAHs in soil, surface water and sediment; and the fate after uptake by ecological receptors. The PAHs considered are benzo(a)anthracene, benzo(b)fluoranthene, benzo(k)fluoranthene, chrysene, dibenzo(a,h)anthracene, and indeno(1,2,3-cd)pyrene. Section 2 discusses the environmental fate and transport in soil, surface water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

PAHs strongly adsorb to the soil; therefore, leaching to groundwater and volatilization are slow insignificant processes in most instances (HSDB 1997). However, the persistence of PAHs in soil is dependent upon the number of condensed rings that a PAH contains. The major source of degradation of PAHs in soil is microbial metabolism (ATSDR 1995). Volatilization and photolysis were determined to be important processes for the degradation of PAHs containing less than four aromatic rings, when analyzed from four surface soils amended with PAHs in sewage sludge. However, PAHs containing four or more aromatic rings showed insignificant abiotic losses (Wild and Jones 1993).

Within aquatic systems, PAHs are found sorbed to particles suspended in the water column or particles which have settled to the bottom. This is due to the low solubility and high affinity PAHs have for organic carbon. Studies have estimated that two-thirds of PAHs found in aquatic systems are in particle form and

only one-third are in dissolved form (Eisler 1987). Low molecular weight PAHs (2 to 3 rings) studied in estuaries show that the primary removal processes are volatilization and biodegradation, while high molecular weight PAHs (4 or more rings) volatilize and adsorb to suspended sediments (Thomas 1982; Southworth et al. 1978; Southworth 1979).

Photo-oxidation, chemical oxidation, and biodegradation by aquatic microorganisms are the primary degradation processes associated with PAHs in water (Neff 1979). The process of photo-oxidation varies widely among PAHs when considering the rate and extent of degradation. Benzo(a)pyrene is the most resistant to photo-oxidation, while benzo(a)anthracene is the most sensitive (Neff 1979). Microbial degradation of PAHs in water is very rapid under oxygenated conditions, but extremely slow under anoxic conditions (Neff 1979).

3.0 FATE IN ECOLOGICAL RECEPTORS

Sources of PAH accumulation in aquatic organisms include water, sediment, and food. Bioconcentration factors can range from low to very high, depending on the PAH and the receptor. Invertebrates and bottom-dwelling fish may accumulate PAHs through ingestion of sediment (Eisler 1987).

Studies indicate that fish are capable of metabolizing PAHs by the mixed function oxidase (MFO) system in the liver. The breakdown products are then eliminated through the urine and feces. Half-lives ranging from 2 to 9 days have been reported for the elimination of PAHs in fish (Niimi 1987). Chrysene has a near-surface half-life computed for sunlight at latitude 40°N of 4.4 hours (Zepp and Schlotzhauer 1979). Assimilation of PAHs from contaminated food is readily achieved by fish and crustaceans; however, this process is limited for mollusks and polychaete worms (Eisler 1987). It is also noted that aquatic organisms such as phytoplankton, certain zooplankton, mussels, scallops, and snails lack a metabolic detoxification enzyme system. Therefore, these organisms have potential for PAH accumulation (Malins 1977).

PAHs can be introduced into mammals through ingestion, inhalation, and dermal exposure. Because PAHs are highly lipid soluble and can cross epithelial membranes, they are readily absorbed from the gastrointestinal tract and lung (HSDB 1997). PAHs are absorbed through the mucous lining of bronchi when inhaled (Bevan and Ulman 1991) and taken up by the gastrointestinal tract in fat-soluble compounds when ingested. Passive diffusion is the process in which PAHs are distributed following percutaneous

absorption (Ng et al. 1991). Once absorbed into the body, PAHs are distributed to the lymph fluid and then the blood stream. Following oral or inhalation exposure, PAHs are widely distributed in animal tissue (Bartosek et al. 1984; Withey et al. 1991; Yamazaki and Kakiuchi 1989).

PAHs have limited transfer across the placenta; therefore, PAH levels are generally lower in the fetus, when compared to maternal levels (Neubert and Tapken 1988; Withey et al. 1992). The major metabolism sites for PAHs are the liver and kidneys. Additional sites of metabolism include the adrenal glands, testes, thyroid, lungs, skin, sebaceous glands, and placenta (Meditext 1997). PAHs are primarily excreted through the urine and bile (Bevan and Weyand 1988; Grimmer et al. 1988; Petridou-Fischer et al. 1988; Weyand and Bevan 1986; Wolff et al. 1989).

PAHs may be taken up by terrestrial plants from the soil or air depending on the concentration, solubility, and molecular weight of the PAHs. Lower molecular weight PAHs are absorbed by plants more readily than higher molecular weight PAHs (USFWS 1987). Some plants are capable of producing benzo(b)fluoranthene (HSDB 1997). The partitioning of PAHs between vegetation and the atmosphere was found to be primarily dependent upon the atmospheric gas-phase PAH concentration and the ambient temperature, when studied throughout the growing season under natural conditions (Simonich and Hites 1994). Above-ground parts of vegetables have been found to contain more PAHs than underground parts, mainly attributable to airborne deposition and subsequent adsorption (USFWS 1987). Growth promoting effects were observed in higher plants, as well as cultures of lower plants, when benzo(a)anthracene, indeno(1,2,3-cd)pyrene, and benzo(b)fluoranthene were tested in a series of soil and hydrocultures (Graf and Nowak 1968).

Information was not available on the fate of PAHs in exposed birds.

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POLYCHLORINATED BIPHENYLS (PCBs)

1.0 SUMMARY

Polychlorinated biphenyls (PCB) are mixtures of different congeners of chlorobiphenyl. PCBs are a group of highly fat-soluble, semi-volatile compounds that readily bioaccumulate and biomagnify in ecological receptors, especially upper-trophic-level carnivores in aquatic food webs. In general, PCBs adsorb strongly to soil and sediment, and are soluble in fatty tissues. Volatilization and biodegradation of the lower chlorinated congeners also occur. The toxicological properties of individual PCBs are influenced primarily by: (1) lipophilicity, which is correlated with log K_{ow}, and (2) steric factors resulting from different patterns of chlorine substitution on the biphenyl molecule. In general, PCB isomers with high K_{ow} values and high numbers of substituted chlorines in adjacent positions constitute the greatest environmental concern. Biological responses to individual isomers or mixtures vary widely, even among closely related taxonomic species.

The following is a profile of the fate of PCBs in soil, surface water, and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, surface water, and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

The environmental fate of PCBs in soil depends on the degree of chlorination of the molecule. In general, adsorption and the persistence of PCBs increases with an increase in the degree of chlorination (EPA 1988). Mono-, di-, and trichlorinated biphenyls (Aroclors 1221 and 1232) biodegrade relatively rapidly. Tetrachlorinated biphenyls (Aroclors 1016 and 1242) biodegrade slowly, and higher chlorinated biphenyls (Aroclors 1248, 1254, and 1260) are resistant to biodegradation (HSDB 1997). Although biodegradation of higher chlorinated congeners may occur very slowly, no other degradation mechanisms have been shown to be significant in soil (HSDB 1997). Vapor loss of PCBs from soil surfaces appears to be an important mechanism with the rate of volatilization decreasing with increasing chlorination. Although the volatilization rate may be low, the total loss by volatilization over time may be significant because of persistence and stability of PCBs (Sklarew and Girvin 1987).

In water, adsorption to sediments and organic matter is a major fate process for PCBs (EPA 1988; Callahan et al. 1979). Volatilization of dissolved PCBs is an important aquatic process. Strong PCB adsorption to sediment significantly decreases the rate of volatilization, with higher chlorinated PCBs having longer half-lives than the lower chlorinated PCBs (EPA 1988).

3.0 FATE IN ECOLOGICAL RECEPTORS

Diet is a major route of PCB uptake in many aquatic species (Eisler 1986). However, some species accumulate PCBs from the water column to a much larger extent than the diet, even when comparing closely-related species. Based on its high log K_{ow} value, receptors are expected to bioconcentrate and bioaccumulate PCBs to tissue levels much greater than the concentrations in water and sediment (Eisler 1986). Due to their high lipophilicity, PCBs concentrate mostly in fatty tissues. For upper-trophic-level receptors, diet is the main exposure pathway for PCB exposure (Eisler 1986). In aquatic food webs, evidence indicates that PCBs biomagnify in upper trophic levels, but not in lower trophic levels (Shaw and Connell 1982).

Among mammals, aquatic predators (e.g., mink, otters, seals, etc.) have been found to accumulate PCBs to significant levels. Lower chlorinated PCBs are eliminated more rapidly from lipids than higher chlorinated PCBs. Placental transfer of PCBs occurs in mammals (Hidaka et al. 1983).

The primary biochemical effect of PCBs is to induce hepatic mixed function oxidase systems, increasing an organism's capacity to biotransform or detoxify xenobiotic chemicals. PCBs also induce hepatic enzymes that metabolize naturally occurring steroidal hormones (Peakall 1975). These hepatic microsomal enzyme systems are most likely correlated with observed adverse reproductive effects (Tanabe 1988).

PCBs accumulate in bird tissues and eggs (Eisler 1986). Residues of PCBs in birds are affected by numerous biotic factors including fat content, tissue specificity, sex, and the developmental stage of an organism (Eisler 1986). Sexual differences in PCB bioaccumulation are pronounced due to the female's ability to pass a significant portion of the PCB burden to eggs (Lemmetyinen and Rantamaki 1980).

Water snakes (*Nerodia spp.*) and turtles accumulate PCB levels similar to those of PCB residues in their prey. Aroclor 1260 accounted for most of the PCBs detected in water snakes (Sabourin et al. 1984;

Olafsson et al. 1983). These data suggest diet is an important route of PCB transfer in reptiles (McKim and Johnson 1983).

Organic matter and clay content of soil influences the bioavailability of PCBs to plants (Strek and Weber 1982). Uptake of PCBs from soils by plants has been documented, however, only very low amounts are typically accumulated (Iwata et al 1974, Iwata and Gunther 1976, Weber and Mrozek 1979). Effects of PCBs on plants include reduced growth and chlorophyll content, and negative effects on photosynthesis (Strek and Weber 1982).

Terrestrial and aquatic plants bioconcentrate PCBs (Sawhney and Hankin 1984). Aquatic plants also bioaccumulate PCBs from both the water column and sediments. Transfer of PCBs on microparticulate materials to phytoplankton is well documented, as is partitioning from aqueous solution into algal lipids (Rohrer et al. 1982).

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PENTACHLOROPHENOL

1.0 SUMMARY

Pentachlorophenol (PCP) has a strong affinity for soil, with sorption higher at lower pH and with increased organic content. Microorganisms readily metabolize PCP in soil, surface water, and sediment. Photolysis rapidly breaks down PCP in surface water. Ecological receptors will rapidly absorb PCP, but will also rapidly excrete it. Therefore, the potential for bioconcentration and bioaccumulation is only moderate. PCP biomagnification has not been observed.

The following is a profile of the fate of PCP in soil, surface water, and sediment, and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

PCP adsorbs strongly to soil, with adsorption higher in acidic conditions (Callahan et al. 1979). The amount of PCP adsorbed to soil at a given pH also increases with increasing organic content of the soil (Chang and Choi 1974). The half-life of PCP in soil ranges from weeks to months (Ide et al. 1972; Murthy 1979; Rao and Davidson 1982). Photolysis and hydrolysis do not appear to be significant processes of degradation in soil (Ball 1987). In certain soil environments, PCP may volatilize; however, in general, mobility of PCP in soil is limited (Arsenault 1976).

Biodegradation is considered the major transformation mechanism for PCP in soil, with PCP metabolized rapidly by acclimated microorganisms (Kaufman 1978). The main degradation products of PCP in soil are 2,3,7,8-tetrachlorophenol and carbon dioxide (Knowlton and Huckins 1983).

The fate of PCP in water and sediment is heavily dependent upon the pH of the water. At lower pH, more of the PCP dissociates and is available for degradation (Weiss et al. 1982). PCP also adsorbs to sediment more readily under acidic conditions, and is more mobile under neutral or alkaline conditions (Kuwatsuka and Igarashi 1975).

In surface water, photolysis and biodegradation are the predominant transformation processes for PCP (ATSDR 1994). Photolysis occurs mainly at the water surface, with its impact decreasing with increasing depth (Callahan et al. 1979). The reported half-life for the photolysis of PCP is about 1 hour (Callahan et al. 1979). Biodegradation of PCP can occur under both aerobic and anaerobic conditions, with more rapid degradation under aerobic conditions (Pignatello et al. 1983). The greatest biodegradation of PCP was observed in the top 0.5 to 1 cm layer of sediment.

3.0 FATE IN ECOLOGICAL RECEPTORS

The aquatic toxicity of PCP depends on water pH; at low pH, PCP is more lipophilic, with a high potential for accumulation. At alkaline pH, PCP is more hydrophilic, with a decreased potential for bioconcentration (Eisler 1989). Fish and bivalves may moderately bioconcentrate PCP (Makela et al. 1991). Accumulation of PCP in fish is rapid, and occurs primarily by direct uptake from water rather than through the food chain or diet. In fish, PCP residues are found in the liver, gill, muscle, and hepatopancreas. PCP is readily metabolized in the liver and hepatopancreas. (Menzie 1978). Half-lives in tissues are less than 24 hours (Eisler 1989).

In mammals, PCP may be absorbed into the body through inhalation, diet or skin contact (Eisler 1989). The degree of accumulation is small, since PCP is efficiently and rapidly excreted. The highest residuals are found in the liver and kidneys, likely reflecting that these organs are the principal organs for metabolism and excretion (Gasiewicz 1991). Small amounts of PCP have been shown to cross the placenta (Shepard 1986).

Uptake into rice has been demonstrated in a 2-year study under flooded conditions. After a single application of radiolabeled PCP, 12.9% of the application was taken up by the plants within the first year, with the highest levels found in the roots (Eisler 1989).

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THALLIUM

1.0 SUMMARY

In the environment, thallium exists in either the monovalent (thallous) or trivalent (thallic) form. Thallium is chemically reactive with air and moisture, undergoing oxidation. Thallium is relatively insoluble in water, although thallium compounds exhibit a wide range of solubilities. Thallium adsorbs to soil and sediment and is not transformed or biodegraded. In aquatic organisms, thallium is absorbed primarily from ingestion and thereafter bioconcentrates in the organism. In mammals, thallium is absorbed primarily from ingestion and is distributed to several organs and tissues, with the highest levels reported in the kidneys. Thallium exposure in mammals causes cardiac, neurologic, reproductive and dermatological effects. Thallium is taken up by plants and inhibits chlorophyll formation and seed germination.

The following is a profile of the fate of thallium in soil, surface water and sediment; and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, surface water and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

In soil, thallium exists in either the monovalent (thallous) or trivalent (thallic) form, with the monovalent form being more common and stable and, therefore, forming more numerous salts (Hampel 1968). Thallium is reactive with air and moisture, oxidizing slowly in air at 20°C and more rapidly with increasing temperatures (Standen 1967). Moisture increases the oxidation of thallium. Thallium adsorbs to soil and is not transformed or biodegraded (Callahan et al. 1979).

Elemental thallium is relatively insoluble in water (Windholz 1976). However, thallium compounds exhibit solubilities ranging from 220 mg/L to more than 700,000 mg/L (Standen 1967; Weast 1975).

Thallium adsorbs to sediments and micaceous clays (Callahan et al. 1979; Frantz and Carlson 1987). Data regarding the transformation or biodegradation of thallium in water were not located.

3.0 ECOLOGICAL RECEPTORS

The primary exposure route for aquatic organisms exposed to thallium is ingestion. Thallium bioconcentrates in aquatic organisms (Zitko and Carson 1975). Toxic effects have been observed in numerous aquatic organisms including daphnia, fat-head minnow, sheepshead minnow, saltwater shrimp, atlantic salmon, bluegill sunfish, and others (USEPA 1980).

Birds and mammals are exposed to thallium via ingestion of soil, water, and plant material (Lie et al. 1960). Following absorption, thallium is distributed to numerous organs including the skin, liver, and muscle, with the greatest amount found in the kidneys (Downs et al. 1960; Manzo et al. 1983). Thallium is excreted primarily in the urine, with some excretion in the feces (Lehman and Favari 1985). Thallium is distributed from the maternal circulation to the fetus (Gibson et al. 1967; Gibson and Becker 1970). Various effects and toxic responses have been reported. Tikhonova (1967) reported paralysis and pathological changes in the liver, kidneys, and stomach mucosa in rabbits chronically exposed to thallium. Formigli et al. (1986) reported testicular toxicity in rats exposed to thallium. Grunfeld et al. (1963) reported changes in the electrocardiographs of rabbits following oral exposure to thallium.

Some levels of thallium occurs naturally in plants (Seiler 1988). Thallium is taken up by the roots of higher plants (Cataldo and Wildung 1983). Thallium has been shown to inhibit chlorophyll formation and seed generation (OHM/TADS 1997).

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VINYL CHLORIDE

1.0 SUMMARY

Vinyl chloride is a low molecular weight organic compound that rapidly volatilizes after released to soil and surface water. Aquatic organisms may take up vinyl chloride, however it is rapidly depurated because it is highly water-soluble. Routes of exposure for wildlife include inhalation, ingestion, and dermal exposure. Bioaccumulation in terrestrial and aquatic organisms is not an important process in the environmental fate of vinyl chloride because of its high volatility and the rapid metabolism by higher-tropic-level receptors.

The following is a profile of the fate of vinyl chloride in soil, surface water and sediment, and the fate after uptake by ecological receptors. Section 2 discusses the environmental fate and transport in soil, surface water, and sediment. Section 3 discusses the fate in ecological receptors.

2.0 FATE IN SOIL, SURFACE WATER, AND SEDIMENT

Vinyl chloride in dry soil has a very short half-life (less than 1 day) (Jury et al. 1984). Vinyl chloride has a high vapor pressure, indicating rapid volatilization from dry soil surfaces (Riddick et al. 1986; Verschueren 1983). Vinyl chloride is also biodegraded and photolyzed in surface soil (ATSDR 1995; Nelson and Jewell 1993). Vinyl chloride does not adsorb to soil in significant amounts.

Vinyl chloride in surface water has a half-life of a few hours (Thomas 1982). An estimated half-life in fresh water for vinyl chloride of 2.5 hours was reported (Mabey et al. 1981). Vinyl chloride is slightly soluble (Cowfer and Magistro 1983). However, vinyl chloride released to surface water will quickly volatilize, negating other fate processes that might be significant based on physical and chemical parameters.

3.0 FATE IN ECOLOGICAL RECEPTORS

Vinyl chloride is not expected to significantly bioconcentrate in aquatic organisms because it has a very low log K_{ow} value. Bioconcentration and accumulation in aquatic carnivores is not expected because of the

high volatility of vinyl chloride and the rapid metabolism of vinyl chloride by higher-tropic-level organisms (Freitag et al. 1985; Lu et al. 1977).

In mammals, vinyl chloride may be absorbed by the body via inhalation (Bolt et al. 1977; Krajewski et al. 1980; Withey 1976), ingestion (Feron et al. 1981; Watanabe et al. 1976; Withey 1976) and dermal contact (Hefner et al. 1975). It is rapidly absorbed and distributed throughout the tissues following uptake. Because of the rapid metabolism and excretion of vinyl chloride, storage within the body is limited.

Information was not available on the fate of vinyl chloride in birds or plants.

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